HCI MONITOR PHASE II

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At present, the short- and long-term environmental impacts of massive HCl releases from the Space Shuttle and other solid-rocket launches are not well characterized. It is important to measure the atmospheric HCl content in both the vapor and aerosol forms. Spectral Sciences, Inc., (SSI) has developed a combination vapor-aerosol HCl monitor under a Phase II SBIR (Small Business Innovative Research program) contract from the Air Force Engineering Services Center (AFESC), Tyndall AFB, Florida.

The instrument consists of four major components: (1) an air sampling, optical measurement unit; (2) a power supply and analog signal output unit; (3) an analog-to-digital (a/d) converter and timing pulse unit; and (4) a personal computer (PC). An air sample is drawn through an aerosol evaporator which vaporizes the aerosols and releases the dissolved HCl into the gas phase. By turning the aerosol heater on and off, one can determine both the total HCl (aerosol and vapor) and the vapor phase HCl. Data acquisition and analysis are

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controlled by a remotely located PC. A 1000-foot signal cable allows the PC to be located in a bunker or control room and enables real-time monitoring of the concentration measurement.

The device is based on measuring the infrared absorption of gas phase HCl in the $3.4 \mu m$ wavelength region. The measurement approach differs from other infrared devices in that it utilizes a novel infrared light source. In essence, the source consists of HCl in a heated cell which emits the characteristic HCl line spectrum. The primary advantage of using a light source which is spectrally matched to the absorption spectrum, is one of species selectivity. This enables quantitative measurement of very small concentrations in the presence of other species that absorb infrared radiation. The dynamic range of the HCl monitor is $0.1-10^3$ parts per million.

PREFACE

This report was prepared by Spectral Sciences, Inc., Burlington MA 01803-5128, under contract F08635-86-C-0137, for the Air Force Engineering and Services Center, Engineering and Services Laboratory (AFESC/RDVS), Tyndall Air Force Base, Florida 32403-6001.

This final report describes the design and development of a combination vapor-aerosol HCl monitor developed under Phase II of the Small Business Innovative Research Program (SBIR). This work was performed between July, 1986 and June, 1988. The AFESC project officer was Capt Mark D. Smith. The principal research staff at Spectral Sciences included L.S. Bernstein, F. Bien, W.K. Cheng, R.P. Domingue, and S.C. Richtsmeier.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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SECTION I

INTRODUCTION

A. OBJECTIVE

Space Shuttle launches deposit massive quantities of hydrogen chloride (HCl) into the environment (Reference 1). At present, the short- and long-term environmental impacts of the HCl releases are not well characterized, and quantitative monitoring of the transport of the HCl into the areas surrounding the launch site is desirable. Previous models and measurements demonstrated that the amount of HCl deposited on the ground depends on the local meteorological conditions, temperature, humidity, windspeed and direction (References 1-11). Furthermore, the HCl can be found in both the vapor and aerosol (hydrochloric acid droplets) forms. The relative partitioning between the vapor and aerosol forms depends on a variety of factors, such as, the HCl and water vapor partial pressures, temperature, and the concentration and composition of the aerosol nucleation sites. Since the concentrations of the HCl in the vapor and aerosol forms may be quite different. it is necessary to monitor both.

B. BACKGROUND

Several HCl monitors have been previously developed (References 12-16); however, none are capable of monitoring both the vapor and aerosol HCl content in real-time. Spectral Sciences, Inc. (SSI) has developed a combined HCl vapor-aerosol monitor under Phase II SBIR (Small Business Innovative Research program) funding from the Air Force Engineering Services Center (AFESC), Tyndall AFB, Florida. The basic operation of the SSI/AFESC HCl monitor is depicted in Figure 1, and a summary of its key operational specifications is given in Table I. The instrument consists of four major components: (1) an air-sampling, optical measurement unit, (2) a power supply and analog signal output unit, (3) an analog-to-digital (a/d) converter and timing pulse unit, and (4) a personal computer (PC).
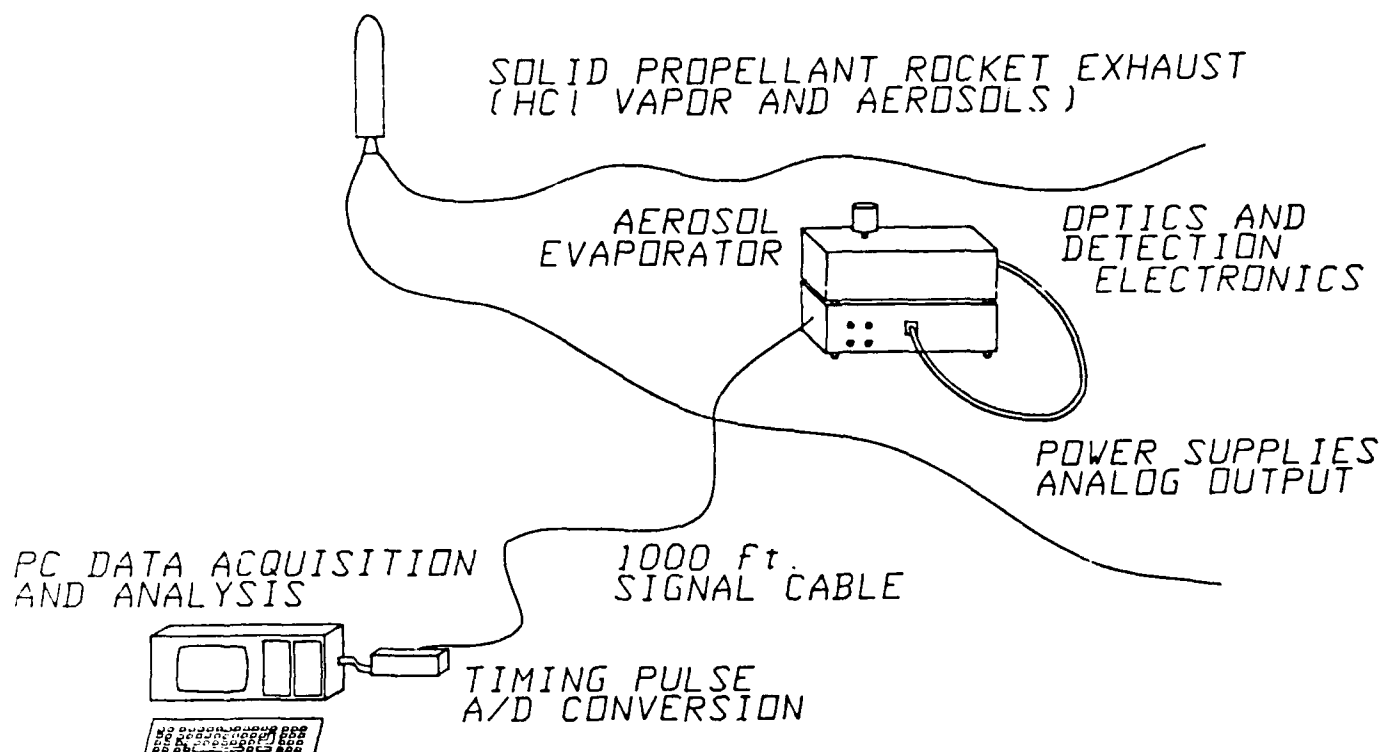
Figure 1.   Schematic of the Operation of the SSI/AFESC HCl Monitor.

TABLE 1.   SPECIFICATIONS FOR THE SSI/AFESC HCl MONITOR.

Minimum Detectable HCl Conc.	100 ppb
Dynamic Range	$0.1 - 10^3$ ppm
Absorption Path Length	7 m (variable from 4-10 m)
Detector	PbSe (cooled to -20 C)
Sample Averaging Time	30 s (variable from $0.1-10^3$s)
Sample Cell Refilling Time	30 s
Electrical Requirements[a]	250 W/120 V AC

(a) This does not include the PC.

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An air sample is drawn through the aerosol evaporator which vaporizes the aerosols and releases the dissolved HCl into the gas phase. By turning the aerosol heater on and off one can determine both the total HCl (aerosol and vapor) and the vapor phase HCl. The HCl concentration measurement is performed with a special infrared light source. Data acquisition and analysis are controlled by a remotely located PC. A 1000 foot signal cable allows the PC to be located in a bunker or control room and enables real-time monitoring of the concentration measurement.

C.   APPROACH

The device is based on measuring the infrared absorption of gas-phase HCl in the 3.4 µm wavelength region. The measurement approach differs from other infrared devices (References 14-16) in that it utilizes a novel infrared light source. In essence, the source consists of HCl in a heated cell which emits the characteristic HCl line spectrum. The primary advantage of using a light source spectrally matched to the absorption spectrum is one of species selectivity. This enables quantitative measurement of very small species concentrations in the presence of strongly absorbing species whose absorption line positions are spectrally uncorrelated with the source line emission.

The basic measurement technique is summarized in Figure 2. The HCl lamp emission consists of high-intensity, narrow HCl emission lines superimposed on a low-intensity continuum. The continuum emission is due to the quartz cell confining the hot HCl gas. Typically, for the HCl lamps produced to date, the total (integrated over wavelength) HCl line emission is approximately equal to the total continuum emission. For a conventional infrared source, such as a continuous black body emitter (heated wire), the total emitted energy within the spectral width of the HCl lines is only around 1 percent of the total black body continuum. This means that the use of the HCl lamp reduces the interference of uncorrelated absorbers by approximately two orders of magnitude.

The HCl monitor uses a single pathlength, gas correlation, spectral filtering scheme. The lamp emission is passed through a filter wheel containing small quartz cells which either contain an HCl/nitrogen mixture

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(designated HCl absorbing) or just nitrogen (designated nonabsorbing). The HCl concentration in the absorbing filter is adjusted to absorb out the HCl line emission. The difference between the total integrated signals for the two filters is equal to the total HCl source line emission. This quantity is determined when no HCl is present in the sample absorption path (White Cell) and is stored in the PC as the "zero" calibration constant. When HCl is introduced into the sample absorption path the difference signal for the two filters is reduced. The difference signal can be quantitatively related to the HCl concentration in the sample path.

The use of a correlated light source in conjunction with gas correlation filtering is a significant improvement over the use of a continuum black-body source with gas correlation filtering. It further reduces, by about two orders of magnitude, the sensitivity of the measurement to uncorrelated absorbers. For example, with conventional gas correlation detection it would be difficult to detect 1 ppm HCl in the presence of 100 ppm CH_4 which also absorbs strongly in the same spectral region as HCl. However, by using the correlated light source it would be
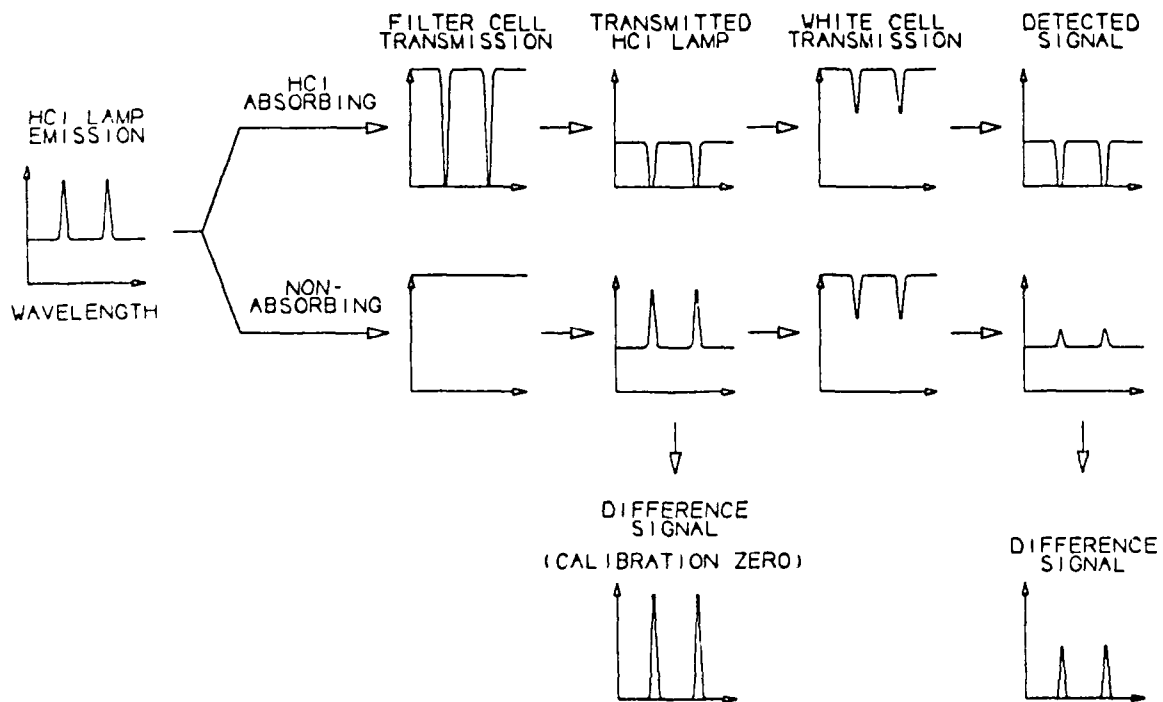
Figure 2. Schematic of Basic Measurement Approach.

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possible to detect 1 ppm HCl in the presence of up to 10,000 ppm CH_4. Another advantage relates to the required accuracy and long-term stability of the zero absorption calibration point. For conventional gas correlation detection the zero calibration must be both accurate and stable to better than 0.01 percent of the absolute signal level to measure an HCl concentration of 1 ppm. However, by using the correlated light source the accuracy and stability of the calibration need be only good to better than 1 percent in order to detect 1 ppm of HCl.

The next section presents an overview of the instrument subsystems and the calibration approach. More detailed discussions on the actual operation and servicing of the HCl monitor are given in the appendices: Appendix A - Instrument Performance Model; Appendix B - HCl Monitor Software; Appendix C - Optical Train; and Appendix D - Electronic Design for the HCl Monitor.

SECTION II

INSTRUMENT DESCRIPTION

A. OPTICAL LAYOUT

The optical layout of the HCl monitor is shown in Figure 3. Light from the HCl lamp is collected by a calcium fluoride lens (25 mm diameter, 50 mm focal length) which focuses the light onto the filter wheel. A second calcium fluoride lens (25 mm diameter, 38 mm focal length) refocuses the light at the entrance aperture to the White Cell (Reference 17). The White Cell mirrors have a focal length of 25 cm, and the effective light collecting diameter of the rear mirrors is 50 cm. The White Cell mirrors were machined out of aluminum blanks which were plated with nickel before polishing and overcoated with gold. The number of passes in the White Cell is adjusted to 28 for a total pathlength of 7 meters. A third calcium fluoride lens (25 mm diameter, 38 mm focal length) refocuses the output of the White Cell onto a thermoelectrically cooled (two-stage) PbSe detector (3mm x 3mm square). A band-pass filter is placed in front of the detector to isolate the most strongly absorbing lines of HCl. The temperature of
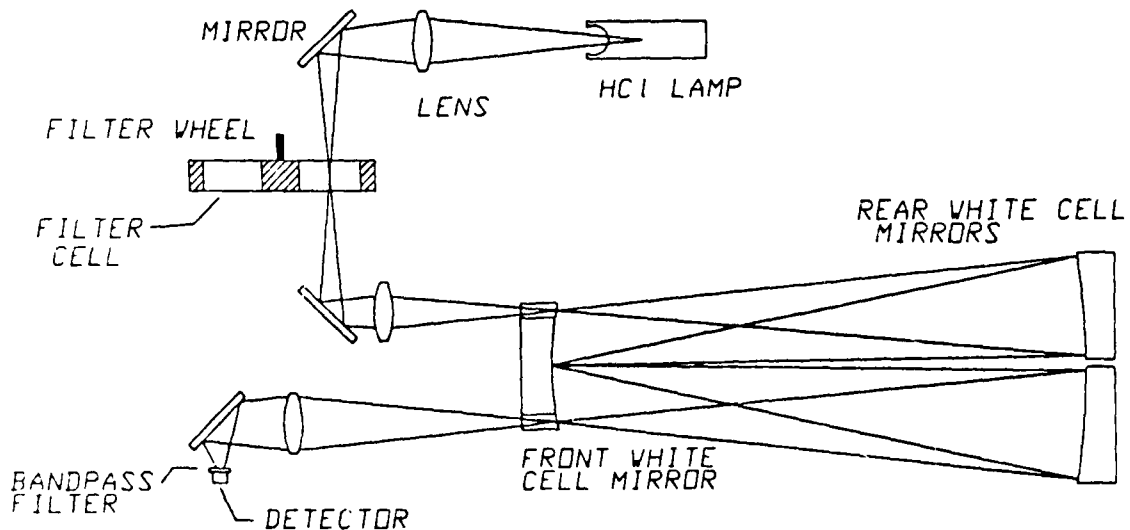
Figure 3. Schematic of HCl Monitor Optical Layout.

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the detector is controlled actively, using a feedback circuit. This circuit uses a thermister built into the detector package to sense the detector temperature and sends a correction current to the thermoelectric cooler, which is proportional to the difference of the actual and preset detector temperatures.

An airtight enclosure is placed over the White Cell (see Figure 4) which allows the air to be drawn through the aerosol evaporator and into the sample absorption path. The sampling pump has a maximum throughput of 94 cc/s and a power requirement of 15 watts. Given the enclosure volume of 2400 cc, it takes about 26 seconds to replenish the sample absorption volume. The replenishing time constant is the fundamental limit to the time response of the HCl monitor to fast changes in the HCl concentration. If a faster response is desired, a higher throughput pump can be used. If one is only interested in the vapor phase HCl, then the White Cell enclosure can be removed and the limiting time response is the time it takes the chopper wheel to make a single revolution (about 0.05 seconds).
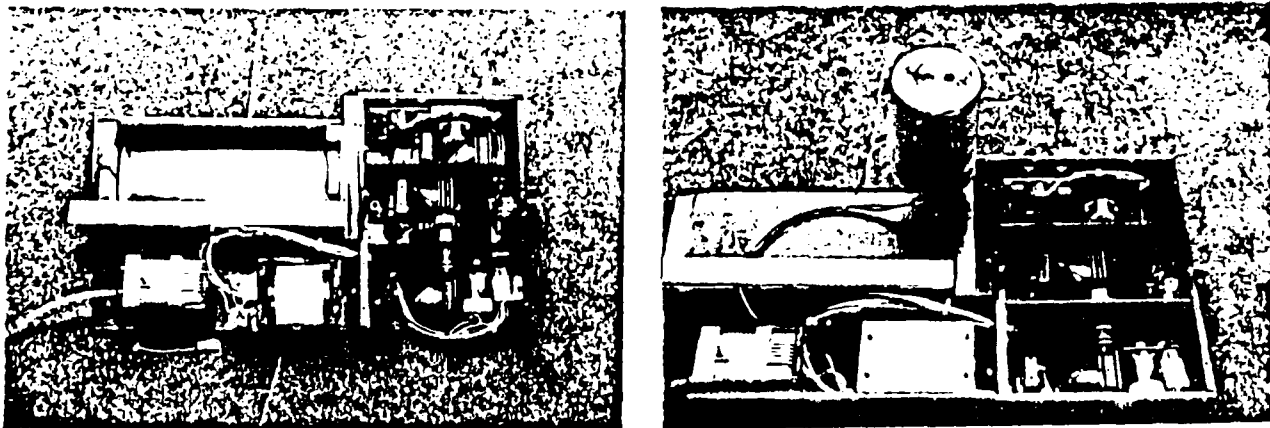
Figure 4. Picture of Optical Components With (Right) and Without (Left) Sample Absorption Path Cover and Aerosol Evaporator.

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B. HCl LAMP

A schematic of the HCl light source is shown in Figure 5. A quartz tube (5.0 cm long by 1.8 cm diameter) is filled with an HCl/nitrogen mixture. The front window of the emission cell is an extremely thin quartz bubble (approximately 0.1 mm thick) developed by G. Finkenbeiner (Reference 18). Because of its thinness this window is very transmissive (see Figure 6) and has a very small emissivity. The thickness of the rear window, 1.5 mm thick quartz flat, is not critical because this part of the cell is not heated. A single layer of insulating material (ceramic fiber paper) is used to separate the cell from the heating wire (26 gauge nichrome). The purpose of this is to more uniformly distribute the heat and background infrared emission from the locally hotter and brighter nichrome wire. About 12 primary nichrome wire "fingers" are spaced uniformly around the cell. These are covered by a layer of insulation and an additional six secondary nichrome "fingers" are used to compensate for radiative and convective losses at the front of the cell. This is important because it prevents the HCl line emission from becoming self-absorbed by the cooler gas near the front window, thus, reducing the sensitivity of the system to small concentrations of HCl in the sample absorption path. The cell is then wrapped with additional insulation to approximately 7 cm diameter. The insulation is baked to drive out all organic binders which increases its insulating properties.

A thermocouple is placed close to the nichrome windings and is used to maintain the cell at constant temperature over a long time. The nominal operating temperature of the lamp is approximately 1000 K, although the exact temperature is not too important as long as it remains constant. The lamp consumes about 12 watts at steady state.

The lamp emission spectrum was measured with a 1/2 meter monochromator and is compared in Figure 7 to model predictions based on the known spectroscopic and radiative transport properties of HCl (References 17-22). From an analysis of the lamp emission spectrum it was determined that the effective emissivity of the quartz was 0.02 and that the integrated

molecular line and continuum emissions over the measurement band pass were nearly equal. The measurement band pass, chosen to select the lamp emission lines which are most strongly absorbed by the much colder atmospheric HCl, is shown in Figure 8.
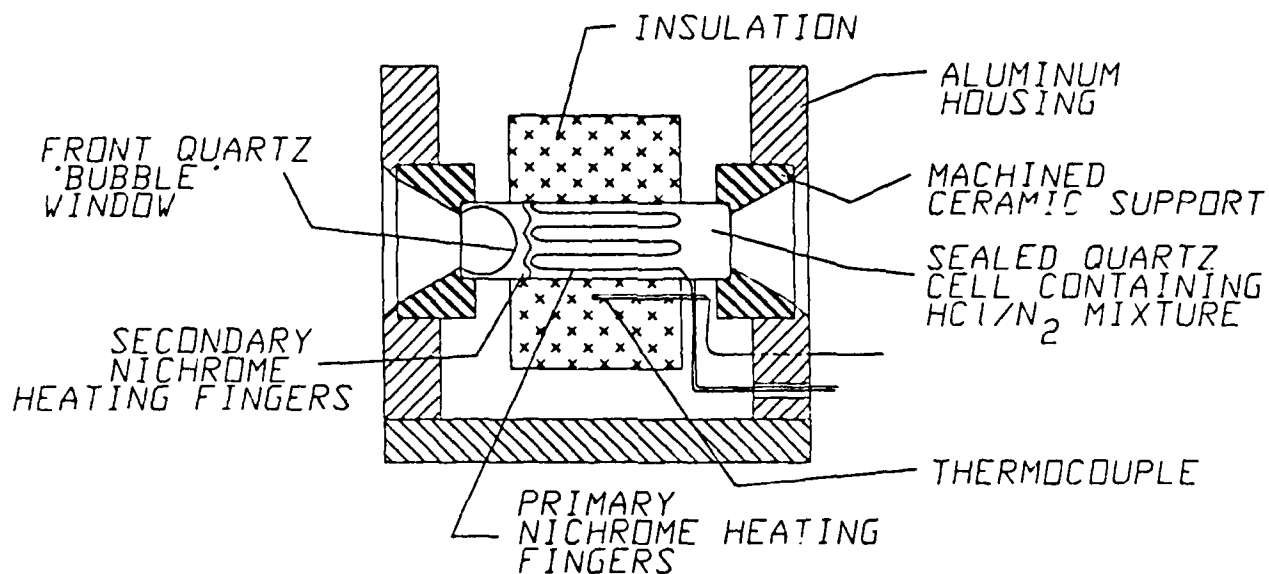
Figure 5. Schematic of the HCl Emission Lamp.
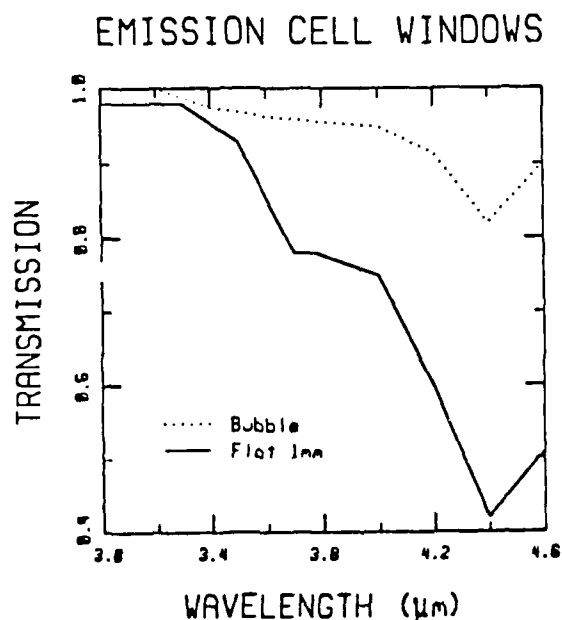
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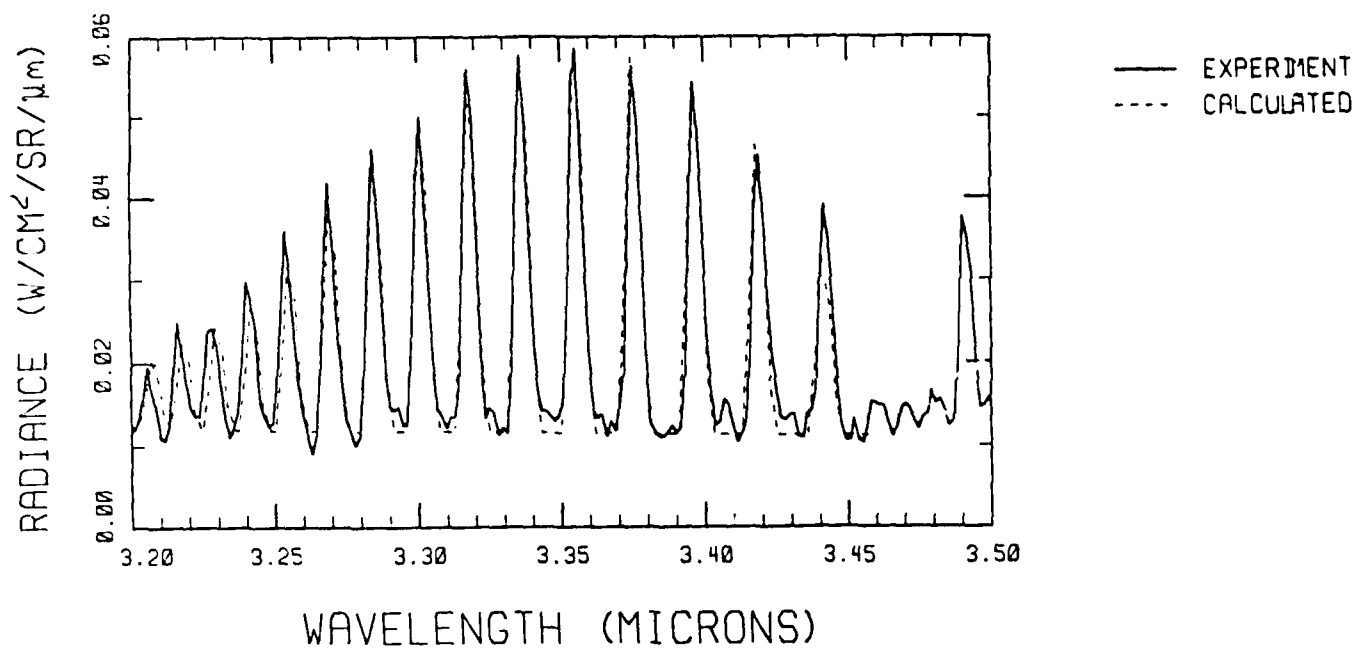
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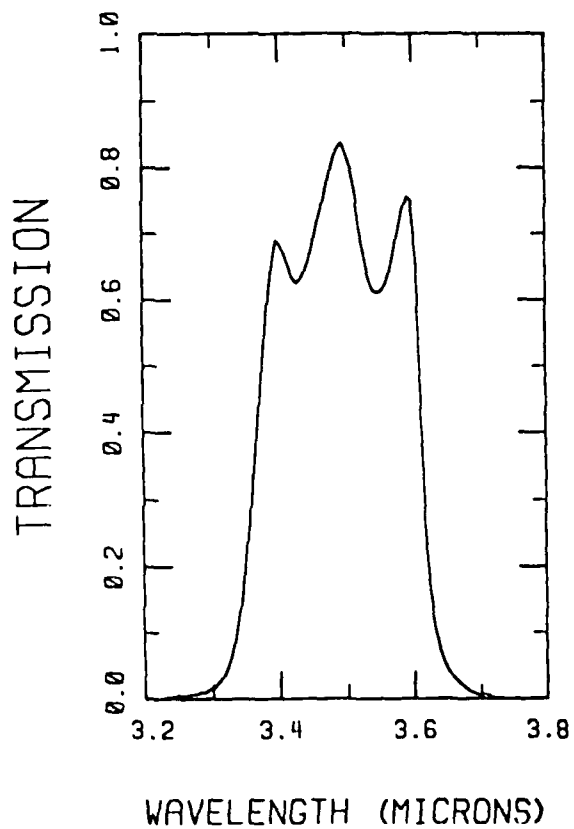
Figure 8. Transmission Spectrum of the Band-Pass Filter.

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C. FILTER WHEEL

The filter wheel and its drive system are shown in Figure 9. It contains four quartz cells (25 mm diameter, 8 mm thick) of which two are filled with dry air and two are filled with an HCl/nitrogen mixture. The concentration of HCl in the filter cell is adjusted so that most of the HCl line emission from the lamp is attenuated. Predictions of the attenuation of the lamp emission for several HCl concentrations in the filter cell are displayed in Figure 10. The current version of the prototype HCl monitor uses an HCl mole fraction of 0.11. The two kinds of cells are arranged so that like cells are 180 degrees opposed. It is not necessary to use a reference pulse to distinguish among the cells or to indicate the overall phase of revolution of the wheel. This is accomplished by the PC signal processing software which recognizes that the signal alternates between just two different maxima with the largest maximum always corresponding to the pure nitrogen filter cell (largest transmission). The filter wheel rotates at 20 revolutions a second; this rate is held constant by a control circuit. This circuit uses a detection output to sense the rotation rate and provides a correction voltage to the motor which is proportional to the difference of the actual and preset rotation rates.
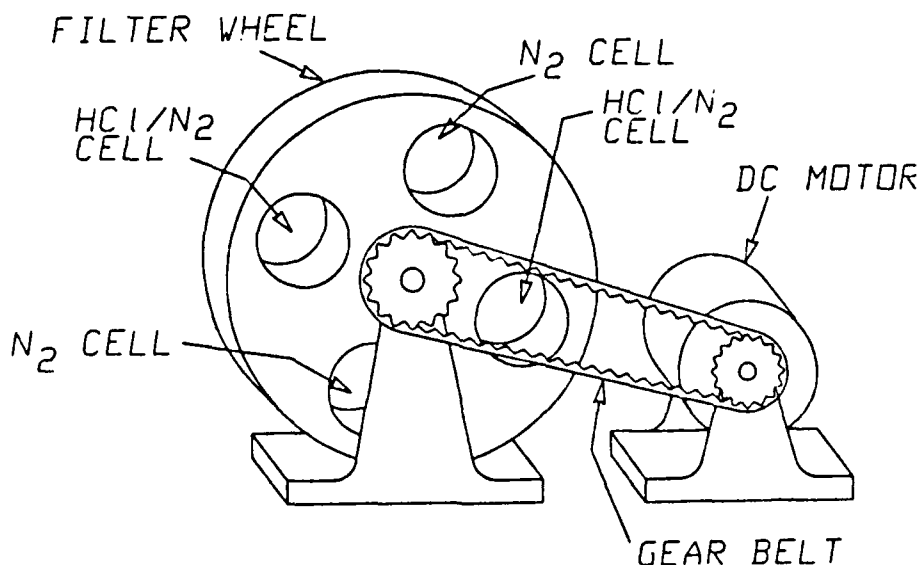
Figure 9. Schematic of Filter Wheel.

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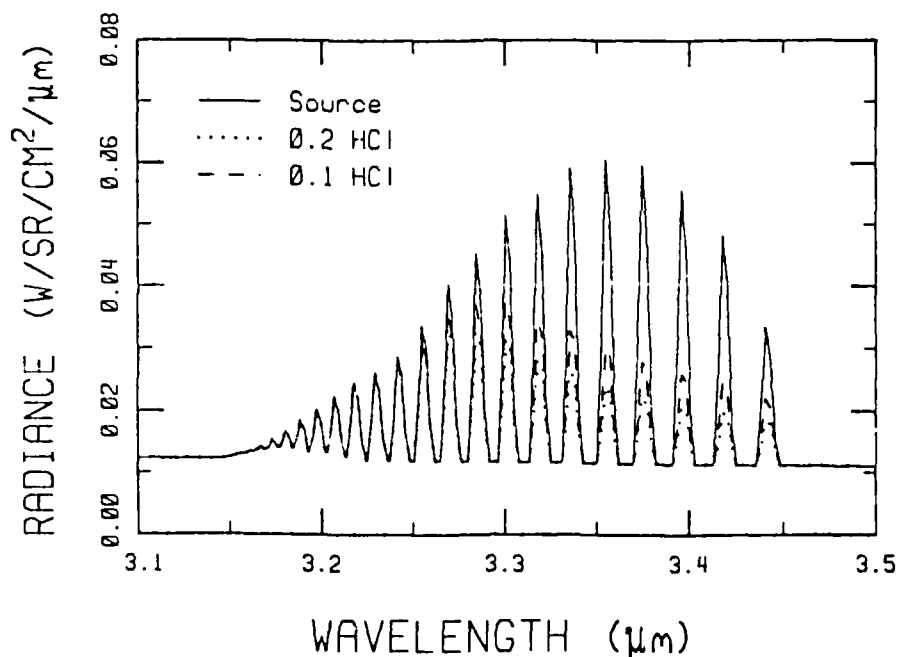
Figure 10. Predicted Attenuation of HCl Lamp Emission for Several HCl Concentrations in the Filter Cell. Filter Cell Conditions: Temperature (295 K), Total Pressure (0.9 atm), and Pathlength (1 cm).

D. SAMPLE CELL TRANSMISSION

The attenuation of the HCl lamp for various concentrations of HCl in the sample cell was experimentally determined using the 1/2 m monochromator at high spectral resolution so that the lines of the individual chlorine isotopes ($H^{35}Cl$ and $H^{37}Cl$) were resolved. This is shown in Figure 11 for one of the absorption lines within the measurement band pass. A 1 cm path length absorption cell was used for these spectral scans. The equivalent concentration for the 7 meter pathlength of the actual instrument is equal to 1/700'th of the concentration in the 1 cm cell. Model predictions, also shown in Figure 11, are in good agreement with the experimental measurements and confirm that even small concentrations of HCl in the sample path can appreciably attenuate the lamp output. About a 1 percent reduction in source intensity occurs for every ppm of HCl in the absorption path. This can be compared to instruments based on a continuum infrared

source, such as the Lawrence Livermore laboratory instrument (Reference 16), where there is approximately a 0.04 percent reduction in source intensity for every ppm of HCl in the absorption path (this assumes a 7-meter total path).
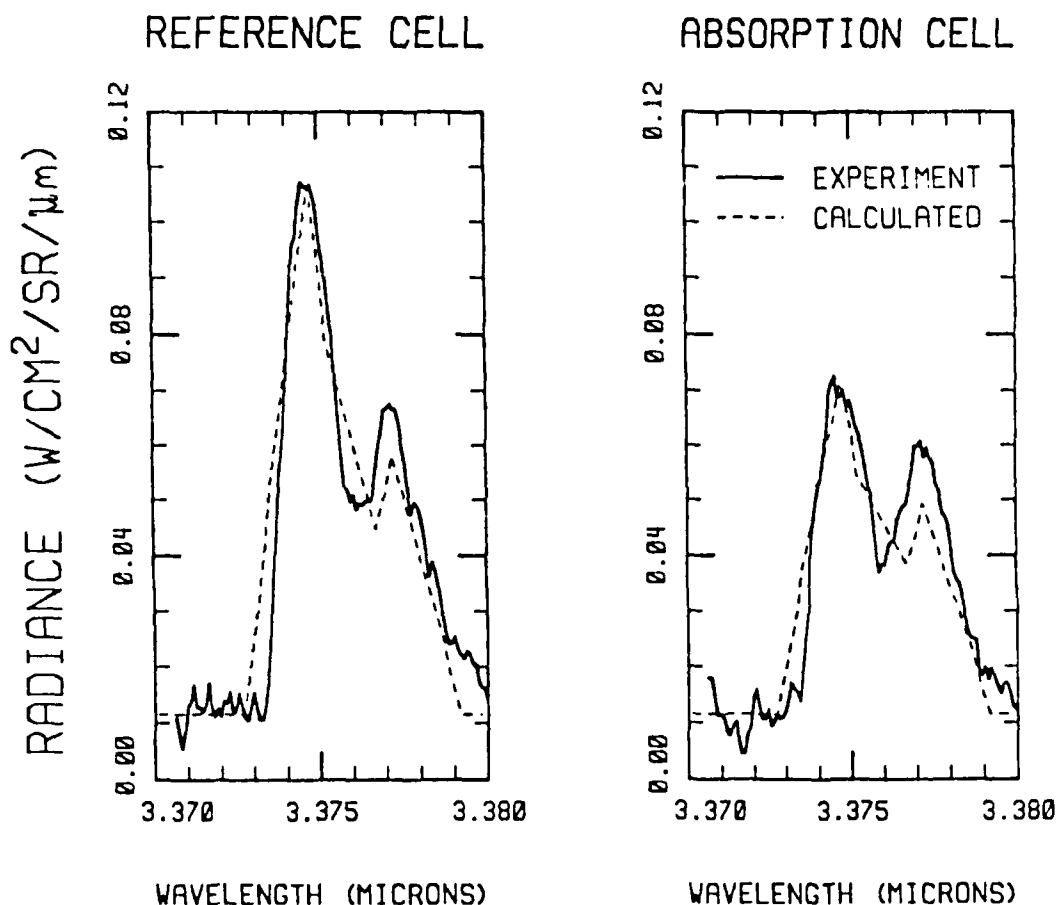
Figure 11. Comparison of Observed and Predicted Attenuation of A Single Pair of Isotopic HCl Emission Lines. Lamp Conditions: Temperature (1100 K), Total Pressure 1.01 atm), Pathlength (4.5 cm), HCl Mole Fraction (0.1), Quartz Emissivity (0.02). Equivalent White Cell Conditions:Temperature (295 K), Pressure (0.92 atm), Path Length (7 m), and HCl Concentration (32.9 ppm).

E. AEROSOL EVAPORATOR

The aerosol evaporator is displayed in Figure 12. Air is drawn through the resistively heated porous carbon plug (2.54 cm o.d, 1.91 cm i.d.). The number of times an aerosol particle encounters the internal surfaces of the carbon plug as it passes through the matrix is determined by the thickness and porosity of the carbon. The total power dissipated by the heater is about 22 watts (4.7 volts through 1.0 ohm).

The steady-state temperature of the gas exiting the heater is 118^{0}C. This temperature is attained in less than 10 seconds after switching on the room temperature evaporator. However, there is a long decay time down to room temperature after the evaporator is switched off. It decays to 54^{0}C in 20 seconds and takes an additional 6 minutes to decay to within 5^{0}C of room temperature. This long decay time is due to the solid carbon base, the metal end caps and the stainless tubing which get quite hot when the evaporator is on and cool slowly by transferring heat to the incoming air after the evaporator is switched off.
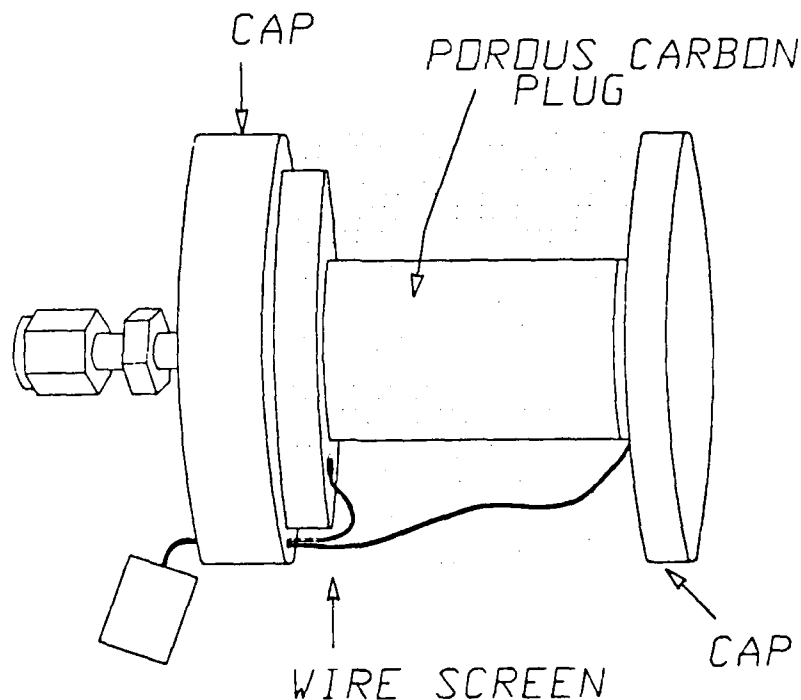
Figure 12. Schematic of the Aerosol Evaporator.

F. DATA ACQUISITION AND SIGNAL PROCESSING

The PbSe detector is operated in a standard ac coupled photo-conductive mode. The detector signal is amplified and buffered to provide a low-impedance signal output, which is proportional to the incident light intensity. To facilitate transmission of the ac signal through the 1000-foot shielded coaxial cable, a 6-volt dc pedestal is added to the detector output. The transmitted signal is again ac coupled to remove the 6-volt bias and the resulting analog signal is shown in Figure 13. A sequence of timing pulses is generated to trigger the a/d converter. The timing pulses are generated using a circuit which outputs a pair of voltage spikes by differentiating the detector signal. Both the time separation of the two spikes and as the time delay of the first spike, relative to the signal leading edge, can be independently controlled. This enables the two spikes to be precisely positioned on the signal curve, one at the *maximum*, and the other at the minimum. Changes in the rotation rate of the filter wheel will cause the timing pulses to occur at positions offset from the maximum and minimum. This is why the rotation rate is controlled.
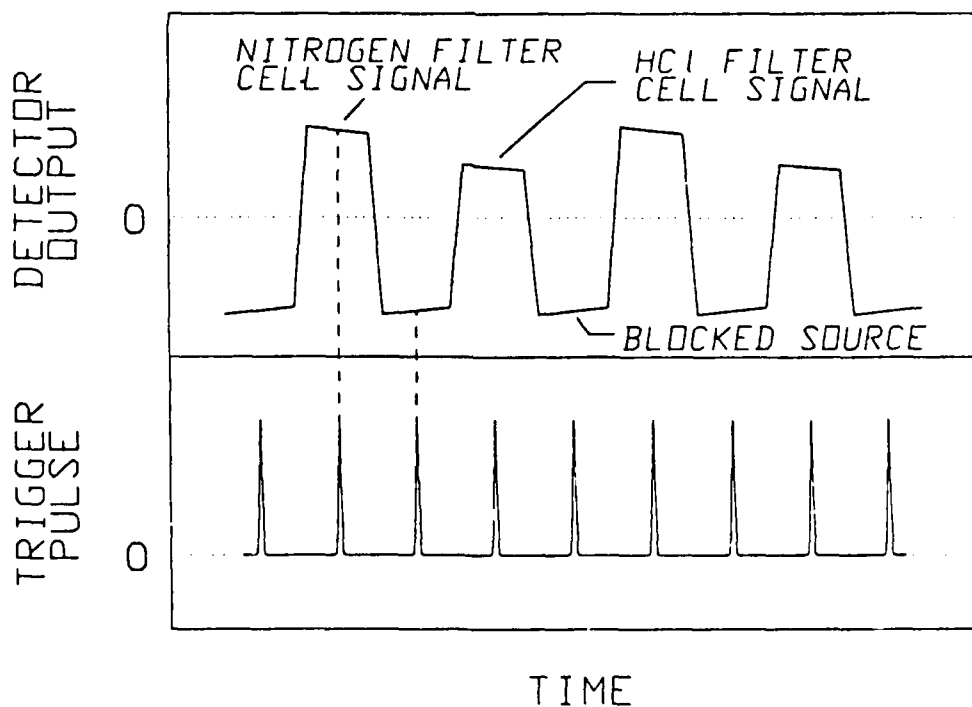
Figure 13. Schematic of Analog Output and A/., Triggering Signals.

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The digitized signals are acquired, processed in real-time, and converted to an HCl concentration using FORTRAN-based software running on an IBM-compatible PC. A difference is taken between each digitized maximum and the average of its adjacent digitized baseline points. This produces two signals, one designated I_a which corresponds to the nitrogen filter and is the most sensitive to HCl absorption in the sample cell, and the other designated I_{na} which corresponds to the HCl filter and is essentially nonabsorbed by the HCl in the absorption path. A ratio of these signals is computed,

$$ r = \frac{I_a - I_{na}}{I_{na}} \quad , \tag{1} $$

where the difference signal is normalized to the nonabsorbing signal. This normalization mitigates the effects of signal drifts caused by fluctuations in the lamp output and accumulation of surface contamination on the White Cell mirrors. An overall system calibration constant, r_0, is determined by measuring the above ratio without HCl in the sample chamber. The concentration of HCl is then related to a normalized ratio,

$$ R = \frac{r}{r_0} \quad , \tag{2} $$

where this quantity is equal to unity for zero HCl concentration and approaches zero for large HCl concentrations. This ratio is actually the average of the ratios for a number of wheel rotations. The number of rotations chosen to be averaged is arbitrary and is selected by the user. Typically, 400 wheel rotations are averaged which takes about 30 seconds and corresponds to the replenishing time of the sample absorption volume.

In determining the HCl concentration from the measured intensity ratio it is convenient to work with the quantity

$$ X = -\ln R \quad , \tag{3} $$

which is proportional to the concentration. In theory (Reference 22) concentration can be related to this quantity via

$$ C = A_1 X + A_2 X^2 \tag{4} $$

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where C is concentration, and A_1, A_2 are coefficients determined by experimental calibration. Higher-order terms can be added if deemed necessary. The effect of temperature on the concentration determination must also be included. Atmospheric temperatures can typically range from around 0° C during the winter to as high as 50^OC on a hot, sunny day in the desert. Also, the aerosol evaporator discharges gas into the sample absorption region at around 118^OC. The effect of temperature can be empirically included in the expansion coefficients through

$$ C = (\frac{T}{T_0})^\alpha C_0 \tag{5} $$

where C_0 is the concentration evaluated at the reference temperature, T_0, and α is a scaling exponent determined from model predictions of the temperature variation.

G. CALIBRATION

The calibration coefficients were determined at room temperature, using known mixtures of HCl in nitrogen which were prepared in a 1 cm pathlength cell. This 1 cm cell was then positioned at the exit of the sample absorption cell and the intensity ratio (as in Equation (2)) was determined. The equivalent concentration in the sample path which would result in this same intensity ratio would be 1/700'th (the ratio of path lengths) of the concentration of the 1 cm cell. By varying the concentration of HCl in the 1 cm cell a large range of equivalent sample cell concentrations were simulated. The HCl concentration in the 1 cm cell was determined by measuring the spectrally resolved transmittance for a black-body light source, then using a synthetic spectral model to match the measured transmittance. An example of the result of this procedure is shown in Figure 14. The calibration curve was determined in two steps. First the inputs to the theoretical model were varied from their nominal values to give a good fit to the calibration points. Then the theoretical curve, which was determined at a much finer grid spacing than the calibration points, was fit to a sixth-order polynomial expansion in X, as in Equation (2). The resulting calibration curve is shown in Figure 15.

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The much larger error bars on the two lowest concentration calibration points reflect the fact that the concentration for these points could not be directly measured. Because their transmittances were too close to unity to yield a measurable absorption loss, the concentrations were estimated by using the relative dilution factor established for the other higher concentration points. The overall accuracy of the calibration is estimated to be approximately ± 20 percent.

The temperature correction exponent was determined by using a first-principles model of the instrument detector output. This model was verified to give good agreement with the experimentally determined room temperature calibration curve and, therefore, can be used with confidence to extrapolate the calibration curve to higher temperatures. Examples of the temperature-dependent calibration curves over the full temperature range of interest are shown in Figure 16. The temperature-dependence is relatively small and is mostly due to the decrease in HCl density at constant pressure as the temperature is increased.
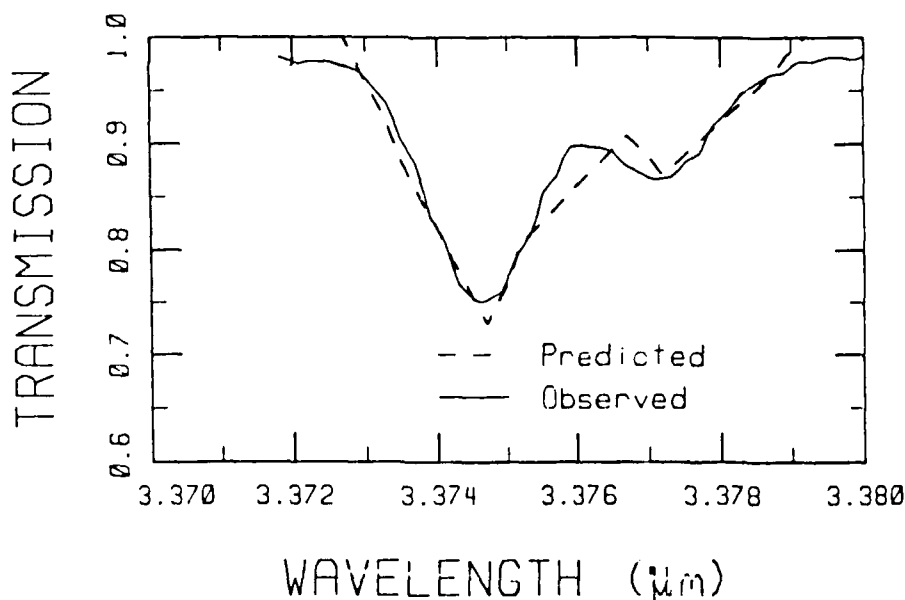
Figure 14.   Comparison of Observed and Predicted Transmission of a Blackbody Source Through an Equivalent Sample Path HCl Concentration of 147 ppm.
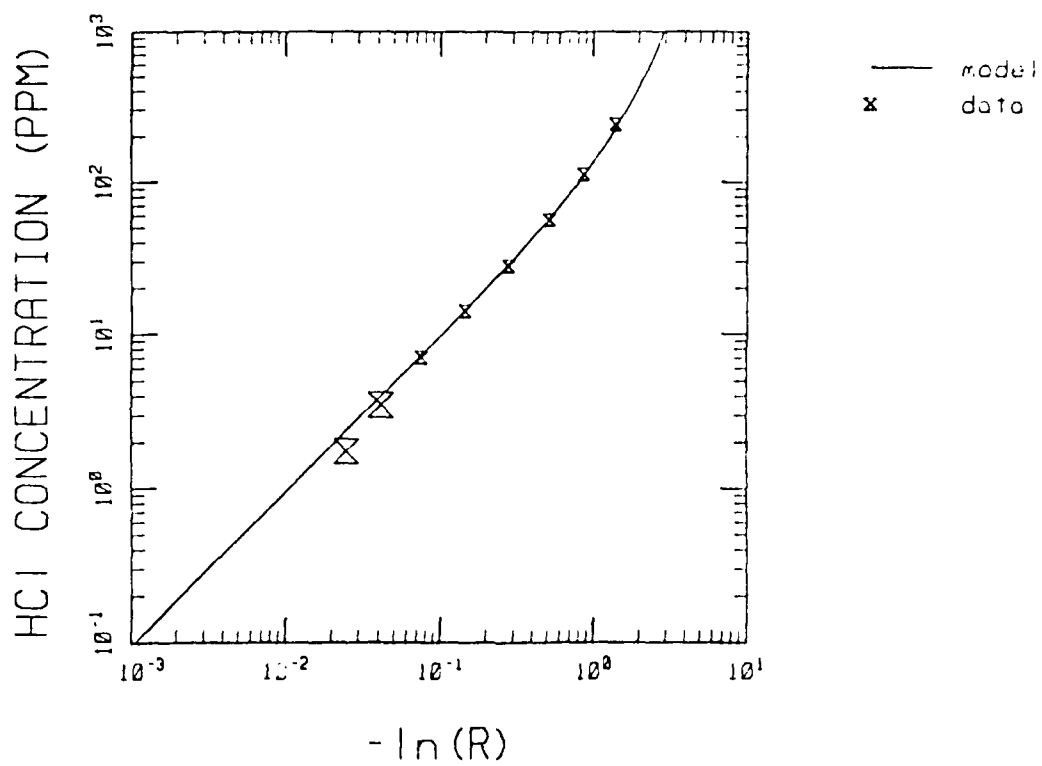
Figure 15. Room Temperature Calibration Curve.
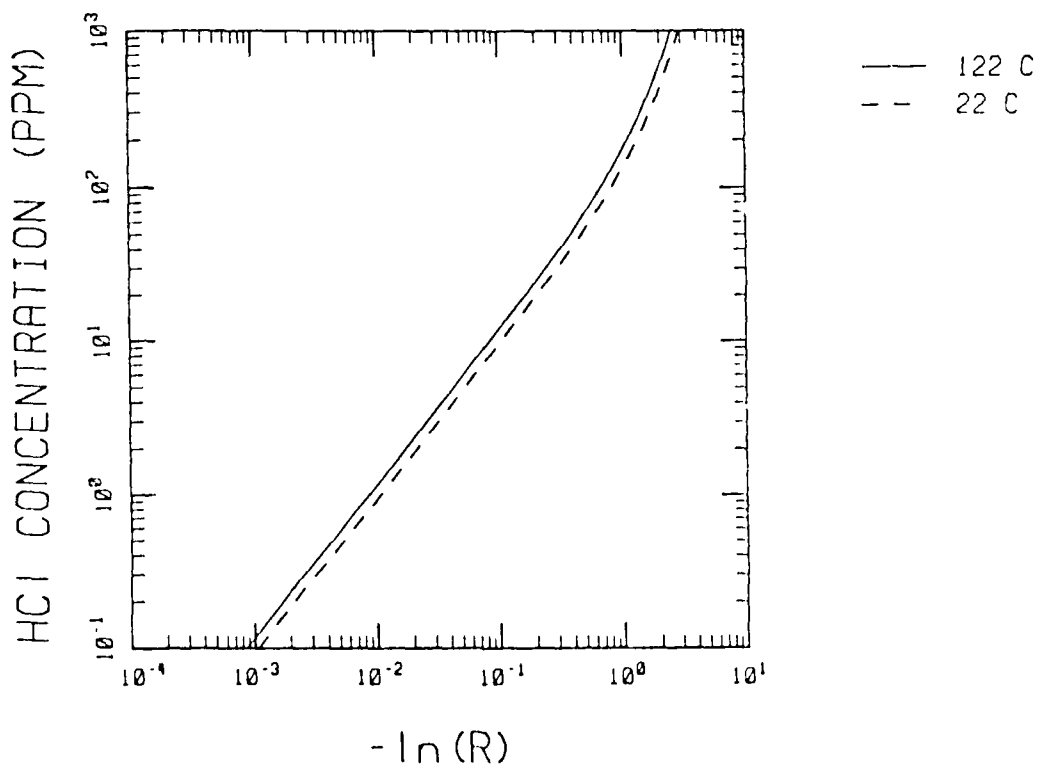
Figure 16. Temperature-Dependence of the Calibration Curve.

An initial test of the instrument was performed using precalibrated mixtures of HCl in nitrogen which were supplied by Matheson. The results are shown in Figure 17. The nominal concentrations for the two mixtures were 61 and 10 ppm. We have found with previous HCl gas mixtures that the concentration can change substantially and unpredictably over long periods of time. The particular mixtures used were about 8 months old so that exact agreement with the nominal concentrations was not expected and the actual results are quite reasonable. The initial measurement points up to approximately 3 minutes were room air samples and indicate the measurement noise for a 15-second measurement average. When the 61 ppm HCl sample was initially turned on there was a large concentration spike. This was due to outgassing from the regulator which had previously been used on a much higher HCl concentration mixture. The concentration decayed rapidly when the HCl sample was turned off at about 22 minutes. The effective evacuation time for the sample absorption cell is around 1 minute which is consistent with the pump throughput. The 10 ppm HCl mixture was turned on at 27 minutes and an initial concentration spike was again observed due to regulator outgassing.
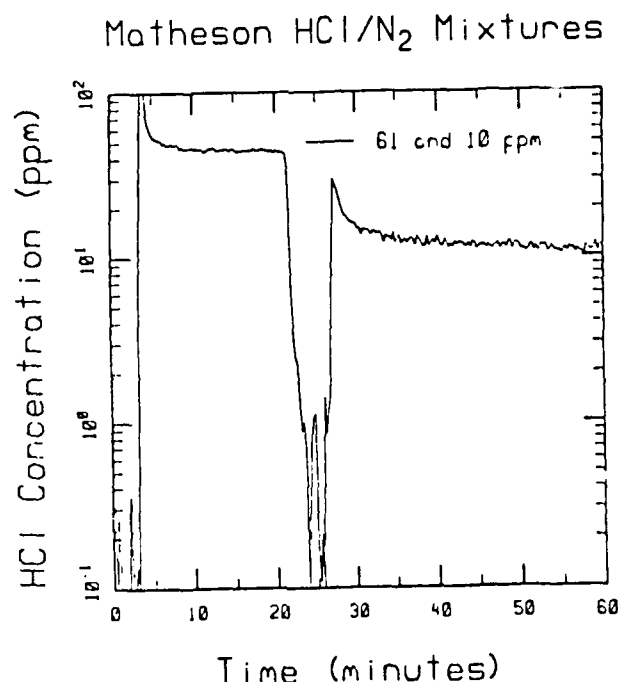
Figure 17. Measurement of Precalibrated Matheson HCl/N_2 Mixtures.

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H. OPERATION AND MAINTENANCE

Operation and maintenance instructions for the HCl monitor are briefly described in this section. Detailed instructions are given in Appendices A-D. The following step-by-step directions are for set up and operation:

- The wooden shipping crate containing the air sampling/optical measurement and power supply modules is placed in the area to be sampled.

- After removing the crate top the aerosol heater and heavy duty extension cord are removed.

- The extension tube for the aerosol heater is attached to the air intake port on top of the optical module.

- The extension cord is connected to the crate fan and power supply power cords.

- Turn the switch for the main power, located on the power supply front panel, to the ON position. A green indicator light will turn on.

- Turn the switch for the aerosol heater, also located on the front panel, to ON. A red indicator light will turn on. The aerosol heater and pump can be controlled remotely from the computer terminal.

- The coaxial signal cable is attached to the front panel of the power supply module.

- The crate top may now be replaced. Pull the two wire cord for the aerosol heater through the opening in the crate top.

- The aerosol heater is attached to the extension tube. This is a Swagelok fitting and should not be excessively tightened.

- The electrical connection to the aerosol heater is made with the polarized two pin connector pulled through the hole in the crate top.

This completes the set up of the sampling unit. The control unit may be remotely located from this module. Its set up is as follows:

- The other end of the coaxial cable is connected to the remotely located PC.

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- The HCl program diskette is loaded into either disk drive and the computer is then turned on.

- After the computer operating system is loaded, it takes about a minute, a prompt,:, will appear on the screen.

- The HCl monitor is then activated by typing "hcl"(ignore quotes) after the prompt.

- A series of questions concerning date file names, data averaging and measurement time period are then answered by the user.

- The results of the measurement are displayed in real time on the screen in the form of a graph of concentration, in units of ppm, versus time.

- The measured data is also placed in a user designated file which can be written to a diskette for permanent storage.

The only routine maintenance required is to check and, if necessary, to clean the White cell mirrors after each field measurement program. Specific instructions for doing this are given in Appendix C. Procedures for changing the calibration constants, replacing the White cell mirrors, realigning the optical system, and adjusting the electronic control circuits are fully detailed in Appendices A-D.

SECTION III

CONCLUSIONS

SSI has successfully developed and tested a novel HCl monitor capable of detecting HCl in both vapor and aerosol phases. An innovative HCl molecular line lamp is used as the light source enabling selective and sensitive detection of HCl. A lower detection limit of 0.1 ppm HCl has been demonstrated with the prototype HCl monitor. The monitor has been delivered to AFESC for use in an ongoing program of monitoring solid propellant firings at several Air Force test and launch facilities.

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APPENDIX A

INSTRUMENT PERFORMANCE MODEL

The detected signal can be expressed by

$$I = \int_{\omega_{min}}^{\omega_{max}} d\omega \tau_f(\omega) \tau_s(\omega) \tau_c(\omega) \{1 - \tau_1(\omega) \tau_w(\omega)\} N(\omega, T_1) \quad , \qquad (A.1)$$

where $\omega(cm^{-1})$ is wavenumber, τ is transmission for the band-pass filter, subscript "f," for the sample cell, subscript "s," for the gas filter cell, subscript "c," for the emission lamp, subscript "1," and for the quartz cell bubble window, subscript "w," and $N(\omega, T_1)(W/sr/cm^2/cm^{-1})$ is the black-body function evaluated at the lamp temperature, T_1. There are frequency independent multiplicative factors such as the collection solid angle which are required to convert the quantity in Equation (A.1) into a quantitative signal level. However, these factors cancel out when signal ratios are used to determine the concentration of the absorbing species in the sample cell. The black-body function is computed from

$$N(\omega, T_1) = \frac{c_1 \omega^3}{\pi \{exp(c_2\omega/T_1) - 1\}} \quad , \qquad (A.2)$$

where $c_1(3.7405 \times 10^{-12})$ and $c_2(1.43879)$ are the first and second radiation constants.

In general, the transmission function for a gaseous absorber can be determined from

$$\tau = exp(-cplk(\omega, T)) \quad , \qquad (A.3)$$

where c is the mole fraction of the absorbing gas, p (atm) is the total pressure, l (cm) is the path length, and k $(cm^{-1} atm^{-1})$ is the frequency and temperature-dependent spectral absorption coefficient. The absorption coefficient for a single molecular line is given by

$$k_j(\omega, T) = \frac{S_j}{\pi \gamma_j} \frac{\gamma_j^2}{(\omega - \omega_j)^2 + \gamma_j^2} \quad . \tag{A.4}$$

where $S_j (cm^{-2}\ atm^{-1})$ is the integrated line strength for the jth line, $\gamma_j (cm^{-1})$ is the line width, and $\omega_j (cm^{-1})$ is the line center location. The total absorption coefficient is found by summing over all the k_j's that contribute to the filter band pass region, and this is the $k(\omega)$ that is used in Equation (A.3).

The line width depends on both temperature and pressure and is calculated from

$$\gamma_j = \gamma_{jf}^0 p \sqrt{T_0/T} + \gamma_{js}^0 cp \frac{T_0}{T} \quad , \tag{A.5}$$

where γ_{jf}^0 is the foreign gas broadening line width, γ_{js}^0 is the self-broadening line width, and $T_0(K)$ is a reference temperature (taken to be at 273 K for the HCl lines). For HCl the line broadening coefficients depend on the particular rotational level associated with the transition and can be approximated by

$$\gamma_{jf}^0 = 0.097 - 7.55 \times 10^{-3} j \quad , \text{ and} \tag{A.6}$$

$$\gamma_{js}^0 = 0.15 - 0.015 j \quad , \tag{A.7}$$

where j is the rotational quantum number of the lower level involved in the transition, γ_{jf}^0 is set equal to 0.014 cm^{-1} for values of j greater than 11, and γ_{js}^0 is set equal to zero for j greater than 10.

The line strength depends on the temperature and is computed from

$$S_m = \frac{\omega_m S_0\{m\} f_m}{\omega_0 q_r(T) qv(T)} \exp\{-c_2 B_0 (m-1)m)/T\} \{1 - \exp(-c_2 \omega_m/T\} \quad , \tag{A.8}$$

where S_0 is the total integrated band strength, $m = j+1$ in the R branch and $m = -j$ in the P branch, ω_0 is the band origin, $\{m\}$ denotes the absolute value of m, ω_m is the transition frequency of the m'th line, f_m is the

Herman-Wallis intensity correction factor, q_r is the rotational partition function, q_v is the vibrational partition function, and B_0(10.6 cm^{-1} for HCl) is the ground state rotational constant. The partition functions are given by

$$q_r(T) = \frac{T}{c_2 B_0}, \text{ and} \qquad (A.9)$$

$$q_v(T) = \frac{1}{1-\exp(-c_2\omega_0/T)} \qquad . \qquad (A.10)$$

The Herman-Wallis factor is given by

$$f_m = 1.-0.025m \qquad . \qquad (A.11)$$

The transition frequencies are determined from

$$\omega_m = \omega_0 + a_1 m - a_2 m^2 - a_3 m^3 \qquad , \qquad (A.12)$$

where the expansion coefficients(a_1, a_2, a_3) and the band center location, ω_0, are different for each isotope of HCl. These values are tabulated below.

	ω_0	a_1	a_2	a_3
$H^{35}Cl$	2886.04	20.5725	0.3072	2.13×10^{-3}
$H^{37}Cl$	2883.92	20.5425	0.3065	2.13×10^{-3}

The integrated line strength for HCl is 155 cm^{-2} atm^{-1} however before using it in Equation (A.8) it must be adjusted to account for the isotopic abundances. Thus for $H^{37}Cl$ use $S_0 = 38.8$ and for $H^{35}Cl$ use $S_0 = 116.2$.

The transmission of the quartz bubble window is given by

$$\tau_w = epx(-x_w) \qquad , \qquad (A.13)$$

where x_w is the optical opacity of the window(typically $x_w=0.02$).

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The detected signal given in Equation (A.1) is determined for four sets of conditions: (1) no HCl in the sample absorption path and the nitrogen containing filter cell in the beam path, designated I_a^0, (2) no HCl in the sample path and the HCl filter cell in the beam path, I_{na}^0, (3) HCl in the sample path and the nitrogen filter cell in the beam path, I_a, and (4) HCl in the sample path and the HCl filter cell in the beam path, I_{na}. The first two signals are used to compute the zero calibration constant via

$$r_0 = \{I_a^0 - I_{na}^0\}/I_{na}^0 \quad . \tag{A.14}$$

In general, this calibration constant depends on the temperatures, HCl concentrations, total pressures, and path lengths of both the HCl lamp and the filter cells. However, for a given instrument all these factors are held constant except for the temperature of the filter cells whose temperature is determined by convective cooling of the optics can. Variations in the ambient temperature will then lead to variations in the filter cell temperature. This is why the zero calibration constant must be determined in real time, just prior to an HCl release. A 10°C temperature variation will lead to approximately a 1 percent shift in the calibration constant and would produce about a 0.7 ppm HCl concentration offset in the calibration curve.

The HCl concentration in the sample absorption path is related to a measured signal ratio, modeled by

$$R = \frac{r}{r_0} \quad , \text{ where} \tag{A.15}$$

$$r = \frac{I_a - I_{na}}{I_{na}} \quad . \tag{A.16}$$

In constructing a calibration curve, it is convenient to work with the quantity

$$X = -\ln R \quad , \tag{A.17}$$

which is proportional to the HCl concentration. A theoretical calibration curve can be constructed simply by computing X as a function of the HCl concentration, C, in the sample absorption path. The resulting curve can be fit with a simple polynomial expansion

$$C = A_1X + A_2X^2 + A_3X^3 + \cdots \quad , \qquad (A.18)$$

where the number of expansion terms depends on the desired accuracy of the fit (typically up to X^6 is required for the current application). The calibration curve is temperature dependent and this can be simply incorporated into the via

$$C = (\frac{T}{T_0})^\alpha C_0 \quad , \qquad (A.19)$$

where C_0 is the concentration evaluated at the reference temperature T_0 and α is a scaling exponent determined from model predictions of the temperature variation. For this application $\alpha = 3/4$ was found to yield good approximation to the temperature dependence.

APPENDIX B

HCL MONITOR SOFTWARE

The HCl monitor is a microcomputer-interfaced instrument whose software is described in this section. As was mentioned previously in the electronics section, two signals enter the DATA TRANSLATIONS analog to digital board. The first signal is the amplified output of the PbSe detector Figure B.1a. The second signal is a clock pulse derived from the first signal which tells the A/D board when to read Figure B.1b. Two files are supplied with the disk, "hcl.exe" and "calib". The later file is the 0 ppm HCl calibration constant read by hcl.exe. This constant is updated each time a calibration run is performed. The former file is the actual HCl monitor data collection calibration, and analysis program. A flowchart for this program is shown in Figure B.2.

Upon entering the program a display identifying the program is flashed to the screen for 3 seconds. Then the user is asked whether or not a calibration run is to be performed and for how long. It is advisable to perform an instrument calibration run for at least 1/2 hour (after the instrument warmup period) before collecting data. This procedure ensures that the appropriate 0 ppm HCl calibration constant will be used in determining the HCl concentrations to be later measured. The calibration procedure should be performed while there is no HCl present. If there is some small (a few ppm) HCl concentration present during calibration then the subsequent measuring period may report relative HCl concentration and not absolute concentration. The calibration constant is stored in the file "calib." at the end of the procedure for later recall during a measurement run.

Following the calibration of the instrument, a measurement run can be performed. After selecting the number of wheel turns to average, the user is prompted for the name of the storage file and the duration of the run. It is suggested that data files be stored on a separate floppy to protect against exceeding disk space on the program disk and hence losing the data. The program opens the data file and stores some user supplied header information in it. Then a graphic display of HCl concentration

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versus time is put on the screen. The program data reduction and analysis occurs in the subroutine "anal01." Essentially this routine takes the difference between the large peaks and the small peaks of Figure B.1.a then divides by the small peaks. These are then averaged over the wheel turns and reported back to the main program as the negative logarithm of this quantity. The main program then relates this logarithm to the HCl concentration using a calibration curve. During the acquisition and analysis the (time, concentration) points are displayed on the screen and output to the data file. At the end of acquisition the file is closed and the program stops. At any time during the data acquisition process the program can be stopped and the file saved by pressing the "escape" key.

A program listing follows in Section B.1. The code is implemented in a mixture of FORTRAN, C, and ASSEMBLER. The FORTRAN modules were compiled using the Microsoft Optimizing FORTRAN compiler version 4.10. The C modules were compiled using the Microsoft QuickC compiler version 1.00. The ASSEMBLER modules were assembled with the Microsoft Macro Assembler version 5.0. The modules were linked with the Microsoft Extended Overlay Linker version 5.01.20 and all software was developed on an IBM PC/XT compatible under the PC-DOS version 3.1 operating system.
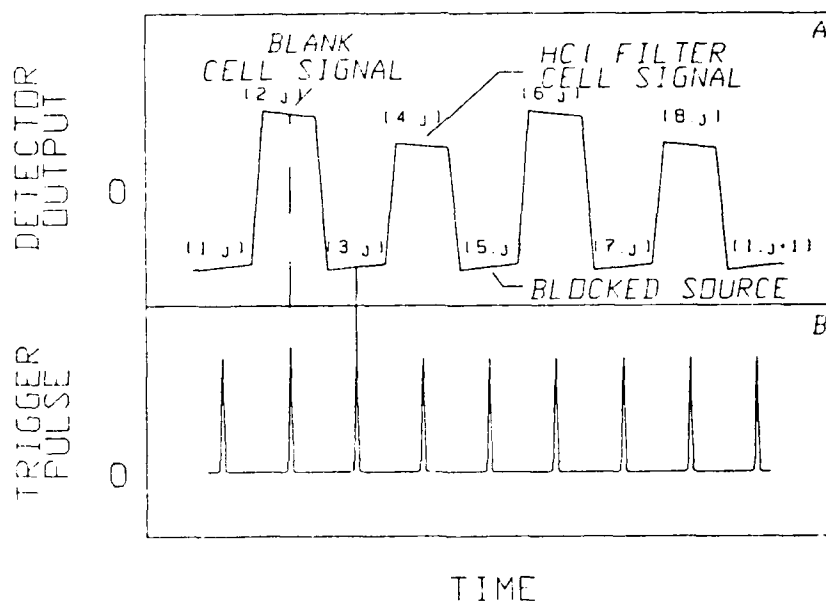
Figure B.1.   Signal Processing for HCl Monitor.
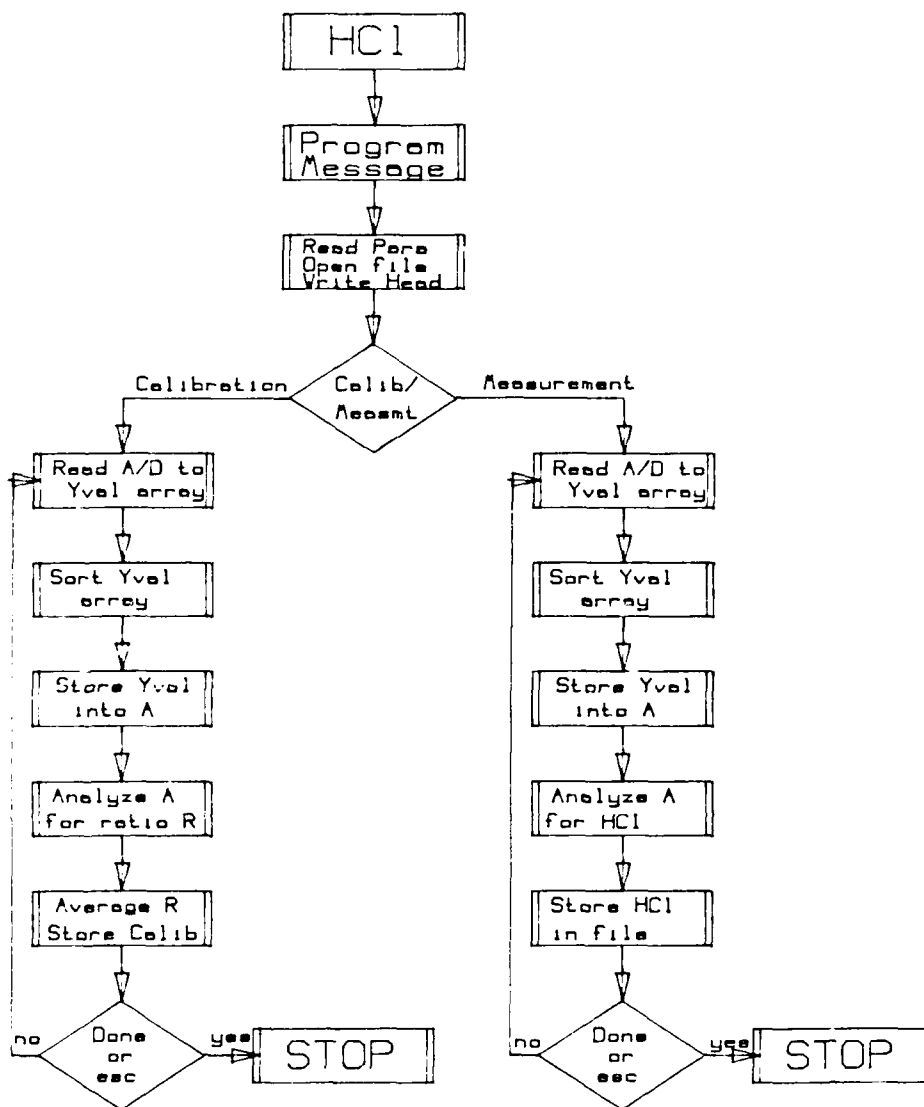
Figure B.2. Flowchart for HCl Program.

```
c
c... Subroutine to analyze the voltage array A from the main
c... HCl program.  The major result is a returned value of X
c... which is related to the HCl concentration in ppm.  If full
c... output is requested, as in a calibration run, then a number
c... intermediate results are displayed to the screen.
c
        subroutine anal01(flag,n,r0,Rtot,X,A)
c
c... A(i,j)  = Array containing the voltage measurements of all
c...            of the wheel turns
c... Ared(i) = peak-null voltage of first peak
c... Bred(i) = peak-null voltage of second peak
c... Cred(i) = peak-null voltage of third peak
c... Dred(i) = peak-null voltage of fourth peak
c... Diff1(i)= (1st peak - 2nd peak difference)/Bred
c... Diff2(i)= (3rd peak - 4th peak difference)/Dred
c... R(i)     = HCl ratio for a single wheel turn
c... sigma(i)= standard deviation of ave(i)
c... ave(i)  = average of the eight measurements, Ared, Bred, Cred, Dred
c...            Diff1, and Diff2 over the number of wheel turns
c... Rtot    = HCl ratio
c... X        = -ln(Ratio) related to HCl concentration
c... n        = number of wheel turns
c... r0       = HCl ratio in the absence of HCl
c
        real*4 A(8,401),Ared(400),Bred(400),Cred(400)
        real*4 Dred(400),Diff1(400),Diff2(400),R(400)
        real*4 sigma(14),ave(14),Rtot,X
        character flag*1
c
        if(.not.(flag.eq.'y'.or.flag.eq.'Y'.or.flag.eq.'n'
     1    .or.flag.eq.'N')) then
```

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```fortran
      print *,'Input error to anal01'
      print *,'Flag must equal "Y" or "N", input flag'
      stop
      endif
      Rtot = 0.0
      do 10 j=1,n
            Ared(j)  = A(2,j) - 0.5*(A(1,j) + A(3,j))
            Bred(j)  = A(4,j) - 0.5*(A(3,j) + A(5,j))
            Cred(j)  = A(6,j) - 0.5*(A(5,j) + A(7,j))
            Dred(j)  = A(8,j) - 0.5*(A(7,j) + A(1,(j+1)))
            Diff1(j) = (A(2,j) - A(4,j))/Bred(j)
            Diff2(j) = (A(6,j) - A(8,j))/Dred(j)
      R(j) = (A(2,j)+A(6,j)-A(4,j)-A(8,j))/(Bred(j)+Dred(j))
      Rtot = Rtot +R(j)
10    continue
      Rtot = Rtot/(r0*float(n))
      if(Rtot.le.0.0) then
         X = 5.0
      else
         X = -alog(Rtot)
      end if
c
      do 100 i=1,8
            ave(i)=0.0
            do 50 j=1,n
                  ave(i)=ave(i)+A(i,j)
50          continue
100   continue
c
      ave(9)=0.0
      ave(10)=0.0
      ave(11)=0.0
      ave(12)=0.0
      ave(13)=0.0
      ave(14)=0.0
```

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```fortran
        do 110 j=1,n
              ave(9)    = ave(9) + Ared(j)
              ave(10)   = ave(10) + Bred(j)
              ave(11)   = ave(11) + Cred(j)
              ave(12)   = ave(12) + Dred(j)
              ave(13)   = ave(13) + Diff1(j)
              ave(14)   = ave(14) + Diff2(j)
110     continue
c
c
        do 200 i=1,8
              ave(i)=ave(i)/float(n)
              sigma(i)=0.0
              do 150 j=1,n
                    sigma(i)=sigma(i)+(A(i,j)-ave(i))**2
150           continue
              sigma(i)=sqrt(sigma(i)/float(n))
200     continue
c
        ave(9)=ave(9)/float(n)
        ave(10)=ave(10)/float(n)
        ave(11)=ave(11)/float(n)
        ave(12)=ave(12)/float(n)
        ave(13)=ave(13)/float(n)
        ave(14)=ave(14)/float(n)
        sigma(9)=0.0
        sigma(10)=0.0
        sigma(11)=0.0
        sigma(12)=0.0
        sigma(13)=0.0
        sigma(14)=0.0
        do 250 j=1,n
              sigma(9)=sigma(9)+(Ared(j)-ave(9))**2
              sigma(10)=sigma(10)+(Bred(j)-ave(10))**2
              sigma(11)=sigma(11)+(Cred(j)-ave(11))**2
```

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```fortran
                  sigma(12)=sigma(12)+(Dred(j)-ave(12))**2

                  sigma(13)=sigma(13)+(Diff1(j)-ave(13))**2

                  sigma(14)=sigma(14)+(Diff2(j)-ave(14))**2

250      continue
c
         do 270 i=9,14

                  sigma(i)=sqrt(sigma(i)/float(n))

270      continue
c
         if(flag.eq.'Y'.or.flag.eq.'y') then
c
         write(6,*)' '

         write(6,*)' '

         write(6,*)'******  Statistics concerning raw data  ******'

         write(6,*)' '

         write(6,111)

111      format(11x,'1',8x,'2',8x,'3',8x,'4',8x,'5',8x,'6',8x,'7',8x,'8')

         write(6,1) (ave(i),i=1,8)

1        format(1x,'ave',3x,F8.5,7(1X,F8.5))

         write(6,2) (sigma(i),i=1,8)

2        format(1x,'sigma',1x,F8.5,7(1X,F8.5))

         write(6,*)' '

         write(6,*)' '

         write(6,*)' '

         write(6,44)

44       format(1x,'******  Statistics concerning four peaks',
     1' and difference ratios  ******')

         write(6,*)' '

         write(6,112)

112      format(1x,9x,'Peak1',7x,'Peak2',7x,'Peak3',7x,'Peak4',
     1 7x,'Diff1',7x,'Diff2')

         write(6,113) (ave(i),i=9,14)

113      format(1x,'ave',3x,F8.5,5(4x,F8.5))

         write(6,3) (sigma(i),i=9,14)

3        format(1x,'sigma',1x,F8.5,5(4x,F8.5))
```

```
c
      write(6,*)' '
      write(6,*)'The smaller difference ratio average is',
   1 amin1(ave(13),ave(14))
      write(6,*)'The larger difference ratio average is',
   1 amax1(ave(13),ave(14))
      endif
      tem1=(ave(13)+ave(14))/2.0
      if(flag.eq.'Y'.or.flag.eq.'y') then
        write(6,*)'The average of averages is',tem1
      endif
      tem1=amin1(ave(13),ave(14))
      tem2=amax1(ave(13),ave(14))
      tem3=(ave(13)+ave(14))/2.0
      return
      end
      interface to subroutine gdate (x)
      integer*4 x
      end
c
      subroutine getdat(month,day,year)
c
c Routine to get the date through an MS-DOS int21H
c function call
c
      integer*4 year,month,day,date
c
      call gdate(date)
c
      year = iand(date,16#FFFF0000)/16#10000
      month = iand(date,16#FF00)/16#100
      day = iand(date,16#FF)
c
      return
      end
```

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```fortran
        interface to subroutine gtime (x)
        integer*4 x
        end
c
        subroutine gettim(hours,minute,second,hundre)
c
c Routine to get the time of day through an MS-DOS int21H
c function call
c
        integer*4 hours,minute,second,hundre,time
c
        call gtime(time)
c
        hours = iand(time,16#FF000000)/16#1000000
        minute = iand(time,16#FF0000)/16#10000
        second = iand(time,16#FF00)/16#100
        hundre = iand(time,16#FF)
c
c       print 101,hours,minute,second,hundre
101     format(1x,i2,':',i2,':',i2,'.',i2)
        return
        end
        interface to subroutine pltgr [c] (x)
        integer*4 x [near, reference]
        end

        interface to subroutine pltpts [c] (x,y,z)
        real*4 x [near, reference]
        real*4 y [near, reference]
        integer*4 z [near, reference]
        end

        interface to subroutine rscrn [c]
        end
```

39

```
      interface to subroutine eschit [c] (x)
      integer*4 x [near, reference]
      end


c
c... This is the main program unit for the SSI HCl monitor
c


      program hcl
c
      real*4 A(8,401),tinit,tfinal,etim,cppm
      real*4 r0,r0a,T
      integer*4 Yval(3208),numave,ngain,lent,mtype,heat
      integer*4 hrs,min,sec,hun,hkey,ncal
      character flag*1,filnam*14
c
c... A(i,j)  = Array in which the measured voltages are stored
c... Yval(i) = Array which contains the integers of the A/D conversions
c... tinit   = Initial time
c... tfinal  = Final time
c... etim    = Elapsed time
c... cppm    = HCl concentration in ppm
c... r0      = Measured ratio in the absence of HCl
c... r0a     = Dummy variable used in calibration
c... T       = Ambient temperature in Celsius
c... numave  = Number of wheel turns to average
c... ngain   = Gain for which the A/D board is set
c... lent    = Length of time for measurement in minutes
c... mtype   = Measurement type, calibration(0) or HCl determination(1)
c... heat    = Aerosol heater on(1) or off(0)
c... hrs     = Hours
c... min     = Minutes
c... sec     = Seconds
c... hun     = Hundredths of seconds
c... hkey    = Value is 27 is escape key hit, 0 otherwise
```

```
c... ncal      = Increment for calibrtion measurement

c... filnam = File name in which to store measurements

c

c

c... conc is the function which relates the ln of the measured

c... ratio and the ambient temperature to the HCl concentration

c... in ppm

c

      conc(T,X) = ((273.0+T)/295.0)**0.75*(95.08*X + 20.59*X*X +
     & 19.65*x**3 - 1.893*X**4 + 0.3074*X**5 + 0.2290*X**6)

c

c... hclscr sets up the initial screen and holds it for 3 seconds

c

      call hclscr(3.0)

c

c... rdparm is the subroutine which reads all of the user input and

c... relays the information back to the main program

c

      call rdparm(numave,ngain,factor,lent,filnam,r0,mtype,heat,T)

c

c... If mtype=1 then do an HCl measurement

c

      if(mtype.eq.1) then

c

c

c

        call gettim(hrs,min,sec,hun)
        tinit = 3600*hrs + 60*min + sec + hun/100

c

c... pltgr is the subroutine which sets up the graphics screen

c

      call pltgr(lent)

c

c... stpclr, setad, and rdAtoD set up and read the A/D board

c
```

41

```
10       call stpclr
         call setad(ngain,8*numave+7,0,0)
         call rdAtoD(8*numave+7,'e','i',Yval)
c
c... sorter sorts Yval according to the procedure outlined in appendix B
c... of the final report
c
         call sorter(numave,Yval)
c
c... convert Yval to volts array A
c
         do 100  j = 1,numave+1
c
         dc 44 i = 1,8
                 A(i,j) = ((20.0 * Yval(8*(j-1)+i)/4096.0) - 10.0)/factor
44       continue
c
100      continue
c
c... analyze the array A for the ln of the average ratio X
c
         call anal01('n',numave,r0,Rtot,X,A)
         call gettim(hrs,min,sec,hun)
         tfinal = 3600*hrs + 60*min + sec + hun/100
         etim = (tfinal-tinit)/60.0
         if(X.ge.5.0) then
            cppm = 10000.0
         else
            cppm = conc(T,X)
         end if
c
c... plot the HCl concentration and store in filnam
c
         call pltpts(etim,cppm,lent)
         write(20,*) etim,cppm
```

```
c
c... check if measurement time is completed or the escape key is hit
c... if yes close filnam and clear and reset screen to text mode
c... if no continue taking data
c
c

      if(etim.ge.float(lent)) then

         close(unit=20)

         call rscrn

         stop

      else

         call eschit(hkey)

         if(hkey.eq.27) then

            close(unit=20)

            call rscrn

            stop

         else

            goto 1G

         endif

      endif
c
c
c

      endif
c
c
c... If mtype=0 then do a calibration measurement
c

      if(mtype.eq.0) then
c
c
c

         r0a = 0.0

         r0 = 1.0

         ncal=1
```

43

```
          print *,'Calibration step'
          print *,' '
c
          call gettim(hrs,min,sec,hun)
          tinit = 3600*hrs + 60*min + sec + hun/100
c
c... stpclr, setad, and rdAtoD set up and read the A/D board
c
20        call stpclr
          call setad(ngain,8*numave+7,0,0)
          call rdAtoD(8*numave+7,'e','i',Yval)
c
c... sorter sorts Yval according to the procedure outlined in appendix B
c... of the final report
c
          call sorter(numave,Yval)
c
c... convert Yval to volts array A
c
          do 200 j = 1,numave+1
c
          do 24 i = 1,8
               A(i,j) = ((20.0 * Yval(8*(j-1)+i)/4096.0) - 10.0)/factor
24        continue
c         write(25,234) (A(i,j),i=1,8)
234       format(1x.8f9.4)
c
200       continue
c
c... analyze the array A for the ln of the average ratio X
c
          call anal01('y',numave,r0,Rtot,X,A)
          call gettim(hrs,min,sec,hun)
          tfinal = 3600*hrs + 60*min + sec + hun/100
          etim = (tfinal-tinit)/60.0
```

```
          cppm = conc(T,X)
c
c... store X in file filnam
c
          write(20,*) etim,X
c
c
c... take runnig average of new r0
c
          r0a = r0a + exp(-X)
          ncal=ncal+1
c
c... check if measurement time is completed or the escape key is hit
c... if yes close filnam, store new r0 in file calib,
c... and clear and reset screen to text mode
c... if no continue taking data
c
c
          if(etim.ge.float(lent).or.ncal.gt.500) then
           close(unit=20)
           r0a = r0a/float(ncal-1)
           rewind(unit=15)
           write(15,*) r0a
           close(unit=15)
           call rscrn
           stop
          else
           call eschit(hkey)
           if(hkey.eq.27) then
              close(unit=20)
              r0a = r0a/float(ncal-1)
              rewind(unit=15)
              write(15,*) r0a
              close(unit=15)
              call rscrn
```

```
                  stop
              else
                  goto 20
              endif
            endif
c
c
c
        endif
c
c
c
1000  stop
      end
          interface to subroutine cls
          end
          interface to subroutine pstrng (x)
          character x*81
          end


          subroutine hclscr(second)
c
c ... This subroutine clears the screen and prints the SSI
c ... copyright information and leaves it up for the number
c ... of seconds specified.  Then the screen is cleared
c ... once more.
c
        integer*4 i
        real*4 second
        character c*81,str1*40,str2*40
c
        call cls
c       write(6,'(1x,80(1H*))')
        str1='****************************************'
        c(1:40)=str1
```

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```fortran
          c(41:80)=str1
          c(81:81)='$'
          call pstrng(c)
          str1='*                                   '
          str2='                                    *'
          c(1:40)=str1
          c(41:80)=str2
          c(81:81)='$'
          do 10 i=1,8
c             write(6,'(1x,1H*,78(1H ),1H*)')
              call pstrng(c)
10        continue
          str1='*                          HC1 MO'
          str2='NITOR                          *'
          c(1:40)=str1
          c(41:80)=str2
          c(81:81)='$'
          call pstrng(c)
c         write(6,'(1x,1H*,34(1H ),11HHC1 MONITOR,33(1H ),1H*)')
          str1='*                                   '
          str2='                                    *'
          c(1:40)=str1
          c(41:80)=str2
          c(81:81)='$'
          do 20 i=1,3
c             write(6,'(1x,1H*,78(1H ),1H*)')
              call pstrng(c)
20        continue
c         write(6,'(1x,1H*,19(1H ),40Hcopyright 1988,  Spectral Sciences, Inc.,
c     &   19(1H ),1H*)')
          str1='*                 copyright 1988,  Spe'
          str2='ctral Sciences, Inc.              *'
          c(1:40)=str1
          c(41:80)=str2
          c(81:81)='$'
```

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```fortran
          call pstrng(c)
          str1='*                                          '
          str2='                                          *'
          c(1:40)=str1
          c(41:80)=str2
          c(81:81)='$'
          do 30 i=1,9
c             write(6,'(1x,1H*,78(1H ),1H*)')
              call pstrng(c)
30        continue
c         write(6,'(1x,80(1H*))')
          str1='*****************************************'
          c(1:40)=str1
          c(41:80)=str1
          c(81:81)='$'
          call pstrng(c)
          call twait(second)
          call cls
          return
          end
          interface to subroutine inplb (a,b)
          integer*2 a,b
          end
          interface to subroutine outlb (a,b)
          integer*2 a,b
          end


          SUBROUTINE RdAtoD(nreads,ieclk,ietrig,Yval)
c
c...FORTRAN routine to read the DT-2401 board following A/D setup with
c...'setup'.  The inputs are: number of conversions, flag(i,e) for internal
c...or external clock, and flag(i,e) for internal or external trigger.
c...The output is an array of A/D conversions
c
C
```

48

```
C
C       BSADRS = Base Address
C       CMDREG = Command Register
C       CMDWAI = Command Wait
C       DATREG = Data Register
C       RDWAI  = Read Wait
C       STAREG = Status Register
C       WRTWAI = Write Wait
C       ADL    = Array to hold low Byte of data
C       ADH    = Array to hold high Byte of data
C       EXTCLK = External Clock code
C       EXTRIG = External Trigger code
C

        integer*4 nreads
        integer*4 Yval(3208)
        character ieclk*1,ietrig*1
C
        INTEGER*2 BSADRS,CMDREG,STAREG,DATREG,CMDWAI,WRTWAI
        INTEGER*2 RDWAI,CSTOP,STATUS,EXTRIG,ERROR1,ERROR2
        INTEGER*2 CRAD,ADL(4008),ADH(4008),EXTCLK,COMAND
C
C
10      BSADRS  = 748
        CMDREG  = BSADRS + 1
        STAREG  = BSADRS + 1
        DATREG  = BSADRS
        CMDWAI  = 4
        WRTWAI  = 2
        RDWAI   = 5 .
C
C
        CSTOP   = 15·
        CRAD             = 14
        EXTCLK  = 64
        EXTRIG  = 128
```

```
c
c
c        Check for legal Status Register value.
c

         CALL INPLB(STAREG,STATUS)

c
c

         IF (.NOT.((IAND(STATUS,112)).EQ.0)) GO TO 98

c
c

         COMAND = 0
         if(ieclk.EQ.'E'.OR.ieclk.EQ.'e') COMAND=COMAND+EXTCLK
         if(ietrig.EQ.'E'.OR.ietrig.EQ.'e') COMAND=COMAND+EXTRIG

c

         comand = crad + comand
                 call WAIT(STAREG,CMDWAI,0)
                 call OUTLB(CMDREG,comand)

c

         DO 222 LOOP = 1,nreads
                 CALL WAIT(STAREG,RDWAI,0)
                 CALL INPLB(DATREG,ADL(LOOP))
                 CALL WAIT(STAREG,RDWAI,0)
                 CALL INPLB(DATREG,ADH(LOOP))
222      CONTINUE
c
c        Check for ERROR.
c
         CALL WAIT(STAREG,CMDWAI,0)
         CALL INPLB(STAREG,STATUS)

c
c        I added this line in order to ignore the high 4 bits
c
c

         STATUS = IAND(STATUS,15)

c
```

50

```fortran
        IF(IAND(STATUS,128).NE.0) GOTO 94
C

        DO 333 LOOP = 1,nreads
        Yval(LOOP) = ADH(LOOP)*256 + ADL(LOOP)
        if(Yval(LOOP).GT.32767) Yval(LOOP) = Yval(LOOP) - 65536
333     CONTINUE
C
69      continue
c       WRITE(*,*)' '
c       WRITE(*,*)' '
c       WRITE(*,*) '       READ A/D Operation Complete'
        GOTO 102
C
C       Fatal board error.
C
94      WRITE(*,*) ' '
        WRITE(*,*) 'FATAL       BOARD ERROR'
        WRITE(6,2) STATUS
2       FORMAT(1X,'STATUS REGISTER VALUE IS ',I2,' DECIMAL')
        WRITE(*,*) ' '
        CALL SR9600(CMDREG,STAREG,DATREG,CMDWAI,RDWAI,
     -CSTOP,CERROR,ERROR1,ERROR2)
        WRITE(*,*) 'ERROR       REGISTER VALUES ARE:'
        WRITE(6,3) ERROR1
3       FORMAT(1X,'      BYTE 1 -   ',I2,' DECIMAL')
        WRITE(6,4) ERROR2
4       FORMAT(1X,'      BYTE 2 -   ',I2,' DECIMAL')
        WRITE(*,*) ' '
        GOTO 102
C
C       Illegal Status Register.
C
98      WRITE(*,*) ' '
        WRITE(*,*) 'FATAL       ERROR - ILLEGAL STATUS REGISTER VALUE'
        WRITE(6,5) STATUS
```

```
5        FORMAT(1X,'STATUS REGISTER VALUE IS ',I2,' DECIMAL')
         write(*,*)'failure in 'rdAtoD''
C
102      RETURN
         END
         interface to subroutine inplb (a,b)
         integer*4 a,b
         end
         interface to subroutine outlb (a,b)
         integer*4 a,b
         end


         subroutine setad(GNCODE,NUMCNV,SRTCHN,ENDCHN)
C
         integer*4 STAREG,STATUS,CMDWAI,CMDREG,CSAD,WRTWAI
         integer*4 DATREG,GNCODE,SRTCHN,ENDCHN,BSADRS
         integer*4 NUML,NUMH,NUMCNV
c
c...FORTRAN routine to set the DT-2401 board for the proper A/D gain,
c...number of conversions, start channel, and end channel.  To be called
c...following 'stpclr'
c
C
C
C        BSADRS = Base Address
C        CMDREG = Command Register
C        CMDWAI = Command Wait
C        DATREG = Data Register
C        STAREG = Status Register
C        WRTWAI = Write Wait
C        GNCODE = Gain Code
C
C
10       BSADRS  = 748
         CMDREG  = BSADRS + 1
```

52

```
          STAREG  = BSADRS + 1

          DATREG  = BSADRS

          CMDWAI  = 4

          WRTWAI  = 2

C

C

          CSAD    = 13

C

C

C         Check for legal Status Register value.

C

          CALL INPLB(STAREG,STATUS)

c

c

          IF (.NOT.((IAND(STATUS,112)).EQ.0)) GO TO 98

C

C         Do a SET A/D PARAMETERS command to set up the A/D converter.

C         Write SET A/D PARAMETERS command.

C

          CALL WAIT(STAREG,CMDWAI,0)

          CALL OUTLB(CMDREG,CSAD)

C

C         Write A/D gain byte.

C

          CALL WAIT(STAREG,WRTWAI,WRTWAI)

          CALL OUTLB(DATREG,GNCODE)

C

C         Write A/D start channel byte.

C

          CALL WAIT(STAREG,WRTWAI,WRTWAI)

          CALL OUTLB(DATREG,SRTCHN)

C

C         Write A/D end channel byte.

C

          CALL WAIT(STAREG,WRTWAI,WRTWAI)
```

53

```fortran
      CALL OUTLB(DATREG,ENDCHN)
C
C     Write high and low bytes of NCONVERSIONS#.
C
      NUMH = INT(NUMCNV/256)
      NUML = NUMCNV - NUMH * 256
      CALL WAIT(STAREG,WRTWAI,WRTWAI)
      CALL OUTLB(DATREG,NUML)
      CALL WAIT(STAREG,WRTWAI,WRTWAI)
      CALL OUTLB(DATREG,NUMH)
C
c     write(*,*)' '
c     write(*,*)'SET A/D PARAMETERS completed'
      goto 102
98    WRITE(*,*) ' '
      WRITE(*,*) 'FATAL ERROR - ILLEGAL STATUS REGISTER VALUE'
      WRITE(6,5) STATUS
5     FORMAT(1X,'STATUS REGISTER VALUE IS ',I2,' DECIMAL')
      write(*,*)'failure in "setad"'
C
102   return
      end
      subroutine sorter(n,Y)
c
c...FORTRAN routine to sort the data read from the DT-2401 board so
c...that the first point is a baseline, the second is the first large
c...maximum, the third is a baseline, the fourth is the first small
c...maximum, then a repetition for up to the number of wheel turns
c...specified.
c
c
      integer*4 n,Y(3208),dum,ndum,idum,mdum
c
      dum = max(Y(1),Y(2),Y(3),Y(4),Y(5),Y(6),Y(7))
c
```

```fortran
      mdum = -32767
      do 10 i=1,7
            if(Y(i).EQ.dum) then
                  ndum = i
                  goto 11
            end if
10    continue
c
11    do 12 i=1,7
            if(i.NE.ndum) mdum = max(mdum,Y(i))
12    continue
c
      do 13 i=1,7
            if(Y(i).EQ.mdum.AND.i.NE.ndum) then
                  kdum = i
                  goto 14
            end if
13    continue
c
14    if(ndum.GE.2) then
            do 20 i=1,8*n+1
                  Y(i) = Y(i+ndum-2)
20          continue
            return
c
      else
            if(kdum.GE.2) then
                  do 30 i=1,8*n+1
                        Y(i) = Y(i+kdum-2)
30                continue
                  return
c
            else
                  write(*,*)'*** error in subroutine sorter ***'
                  stop
```

55

```
              end if

          end if
c

          return

          end

          interface to subroutine inplb (a,b)

          integer*4 a,b

          end

          interface to subroutine outlb (a,b)

          integer*4 a,b

          end


          SUBROUTINE SR9600(CMDREG,STAREG,DATREG,CMDWAI,RDWAI,
      -CSTOP,CERROR,ERROR1,ERROR2)
c    This part should be separated into a separate subroutine
c
c...FORTRAN routine to read messages from the DT-2401 board
c
          INTEGER*4 CMDREG,STAREG,DATREG,CMDWAI,RDWAI
          INTEGER*4 CSTOP,CERROR,TEMP,ERROR1,ERROR2
C         Read the Error Register.
C
          CALL OUTLB(CMDREG,CSTOP)
          CALL INPLB(DATREG,TEMP)
C
          CALL WAIT(STAREG,CMDWAI,0)
          CALL OUTLB(CMDREG,CERROR)
C
          CALL WAIT(STAREG,RDWAI,0)
          CALL INPLB(DATREG,ERROR1)
C
          CALL WAIT(STAREG,RDWAI,0)
          CALL INPLB(DATREG,ERROR2)
C
          RETURN
```

```fortran
      END
      interface to subroutine inplb (a,b)
      integer*4 a,b
      end
      interface to subroutine outlb (a,b)
      integer*4 a,b
      end


      SUBROUTINE stpclr
C
C...FORTRAN routine to stop and clear the DT-2401 board
C
C
C
C      BSADRS = Base Address
C      CMDREG = Command Register
C      CMDWAI = Command Wait
C      DATREG = Data Register
C      STAREG = Status Register
C
C
      INTEGER*4 BSADRS,CMDREG,STAREG,DATREG,CMDWAI
      INTEGER*4 TEMP,CCLEAR,CSTOP,STATUS
C
      BSADRS  = 748
      CMDREG  = BSADRS + 1
      STAREG  = BSADRS + 1
      DATREG  = BSADRS
      CMDWAI  = 4 .
C
C
      CCLEAR  = 1 .
      CSTOP   = 15
C
C      Check for legal Status Register.
```

```
C

      CALL INPLB(STAREG,STATUS)
c
c

      IF(.NOT.((IAND(STATUS,112)).EQ.0)) GOTO 98
C

C

C     Stop and clear DT2801.
C

      CALL OUTLB(CMDREG,CSTOP)
      CALL INPLB(DATREG,TEMP)
C

      CALL WAIT(STAREG,CMDWAI,0)
      CALL OUTLB(CMDREG,CCLEAR)
C

c     write(*,*)'STOP and CLEAR completed'
      goto 102
C

C     Illegal Status Register.
C

98    WRITE(*,*)' '
      WRITE(*,*) 'FATAL ERROR - ILLEGAL STATUS REGISTER VALUE'
      WRITE(6,2) STATUS
2     FORMAT(1X,'THE VALUE OF STATUS IS ',I2,' DECIMAL')
C

102   RETURN
      END
      subroutine twait(s)
c
c...FORTRAN routine to wait a certain amount of time (sec) then procede
c

c

      real*4 s,tinit,tfinal
      integer*4 i,n,ihrs,imin,isec,ihun
c
```

```fortran
      call gettim(ihrs,imin,isec,ihun)
      tinit = float(3600*ihrs + 60*imin + isec + 0.01*ihun)
10    call gettim(ihrs,imin,isec,ihun)
      tfinal = float(3600*ihrs + 60*imin + isec + 0.01*ihun)
      if((tfinal-tinit).lt.s) goto 10
      return
      end
      interface to subroutine inplb (a,b)
      integer*4 a,b
      end


      subroutine wait(addres,n,m)
c
c...FORTRAN routine to suspend execution until a specified bit pattern
c...is read from the specified port
c
      integer*4 addres,value
      integer*4 result,n,m
1     call inplb(addres,value)
      result = IEOR(value,m)
      result = IAND(result,n)
      if(result.eq.0) go to 1
      return
      end
c
c... Subroutine to read all of the user supplied parameters for the HCl
c... program.
c
      subroutine rdparm(numave,ngain,factor,lent,filnam,r0,mtype,heat,T)
c
c... numave  = Number of wheel turns to measure over
c... ngain   = Gain of A/D board
c.  factor   = Division factor based on ngain for voltage conversion
c... lent    = Time length for measurement run
c... filnam  = Name of user supplied file to store HCl concentrations
```

```
c... r0      = HCl ratio in absence of HCl absorption

c... mtype   = Measurement type: 0 for calibration, 1 for HCl determination

c... heat    = Aerosol heater on(1) or off(0)

c... T       = Ambient temperature in Celsius

c

        integer*4 numave,ngain,lent,mtype,heat

        real*4 r0,factor,T

        character filnam*14,header*72

c

        write(6,*)'Average over how many measurements '

        read(5,*) numave

c33     write(6,*)'select gain factor:'

c       write(6,*) '(0 for   q10 V)'

c       write(6,*) '(1 for    q5 V)'

c       write(6,*) '(2 for  q2.5 V)'

c       write(6,*) '(3 for q1.25 V)'

c       write(6,*)'gain factor:  '

c       read(5,*) ngain

c       if(ngain.LT.0.OR.ngain.GT.3) then

c               write(6,*)' '

c               write(6,*)'Please       input a number between 0 and 3'

c               goto 33

c       end if

        ngain=2

        write(6,*)' '

        if(ngain.eq.0) factor=1.0

        if(ngain.eq.1) factor=2.0

        if(ngain.eq.2) factor=4.0

        if(ngain.eq.3) factor=8.0

c

5       write(6,*)'Name the file you wish to store data to'

11      format(A1)

12      format(A14)

13      format(A72)

14      format(ix,A72)
```

60

```
c
      write(6,*)'filename='
      read(5,12) filnam
      write(6,*)'print a one line header'
      read(5,13) header
      open(20,file=filnam,status='unknown')
      write(20,14) header
c
      mtype = -1
50    write(6,*) 'Measurement type'
      write(6,*) 'Calibration = 0'
      write(6,*) 'HCl testing = 1'
      read(5,*) mtype
      if(.not.(mtype.eq.0.or.mtype.eq.1)) goto 50
      heat=-1
55    write(6,*) 'Aerosol measurement'
      write(6,*) 'Aerosol Heater off = 0'
      write(6,*) 'Aerosol Heater on  = 1'
      read(5,*) heat
      write(6,*) 'Input the ambient temperature in Celsius'
      read(5,*) T
      if(.not.(heat.eq.0.or.heat.eq.1)) goto 55
      write(6,*) 'Input time duration of data accumulation'
      read(5,*) lent
      open(unit=15,file='calib',status='old')
      if(mtype.eq.1) read(15,*) r0
      return
      end
#include <stdio.h>
#include <conio.h>
#include <ctype.h>


/*  This C function checks whether or not the escape key was hit
    yes then 27 (ascii representation of escape key) is returned
    no 0 is returned  */
```

```c
/*  called as FORTRAN subroutine 'eschit(dum)'

    integer*4 dum  */


void eschit(dum)

int near *dum;


{

int c;
   if ( kbhit() ) {

      c = getch();

   }

   else {

      c = 0;

   }

   if (c==toascii(27))  *dum = 27;

   if (c!=toascii(27))  *dum = 0;

}
#include <stdio.h>

#include <ctype.h>

#include <graph.h>


struct videoconfig vc;  /* variable vc of type videoconfig */


void pltgr(tmax)

int near *tmax;  /* tmax is the time scale (min) maximum */


/*  This C function sets up the plotting coordinates for the HCl

    real time measurements.  Used with 'pltpts' to plot the points  */

/*  called as FORTRAN subroutine 'pltgr(tmax)'

    integer*4 tmax  */


{

   int i,J,tkval;
        _setvideomode (_HRESBW);
```

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```c
_getvideoconfig (&vc);
_setcolor (2);
_moveto (52,172);
_lineto (640,172);
_moveto (52,172);
_lineto (52,0);
_moveto (50,0);
_lineto (54,0);
_moveto (50,43);
_lineto (54,43);
_moveto (50,86);
_lineto (54,86);
_moveto (50,129);
_lineto (54,129);
tkval = (*tmax+10)/10;
for (i=52; i<=632; i=i+58) {
    _moveto (i,170);
    _lineto (i,174);
}
_settextposition(1,3);
printf("1000");
_settextposition(6,4);
printf("100");
_settextposition(11,5);
printf("10");
_settextposition(17,6);
printf("1");
_settextposition(22,5);
printf(".1");
_settextposition(23,7);
printf("0");
_settextposition(10,1);
printf("HCl");
_settextposition(11,1);
printf("ppm");
```

```c
        for (i=1; i<=10; i++ ) {
            _settextposition ( 23,(7*(i+1)) );
            printf (d",(tkval+(i-1)*tkval) );
        }
        _settextposition(25,35);
        printf ("time (min)");
}
#include <stdio.h>
#include <math.h>
#include <graph.h>

struct videoconfig vc;  /* variable vc of type videoconfig */


/*  This function accepts the elapsed time and the concentration in
    ppm and plots it on a log plot, tmax is the time scale (min)
    maximum  */
/*  This C funtion plots properly in the _HRESBW mode and should be
    used with "pltgr"  */
/*  called as FORTRAN subroutine "pltpts(etim,cppm,tmax)"
    real*4 etim,cppm
    integer*4 tmax  */


void pltpts(etim,cppm,tmax)
int near *tmax;
float near *etim;
float near *cppm;

{
int xscale;
int x,y;
    xscale = 10*((*tmax+10)/10);
    x = (int) ((548.0* *etim)/xscale);
    if(*cppm <= 0.1)
        y = 0;
    else if(*cppm >= 100.0)
```

64

```c
        y = 172;
    else
    y = (int) (43.0*log10(*cppm)+43.0);
    _setpixel(x+52,172-y);
}
#include <stdio.h>
#include <graph.h>


void rscrn()


/*  This C function clears the screen and sets the video mode to
    _TEXTBW80 (the normal text mode for the Compaq) */
/*  called as FORTRAN subroutine "rscrn" */


{
    _clearscreen(_GCLEARSCREEN);
    _setvideomode(_TEXTBW80);
}
; assembly function to clear the screen, should word in any video mode
; called as FORTRAN subroutine "CLS"


.model large
.code
        PUBLIC  CLS
CLS     PROC
EXTRN   HOME:FAR
        PUSH    BP

        mov     ax,0f00h
        int     010h
        mov     bh,07
        cmp     al,03
        jle     bh_set
        cmp     al,07
        je      bh_set
```

```
        xor     bh,bh
bh_set: mov     ax,0600h
        xor     cx,cx
        mov     dx,184Fh
        int     010h
        call    HOME


        POP     BP
        RET     4
CLS     ENDP
        END
```

; assembly function to position the cursor at the top lefthand corner

; of the screen

; called by assembly function "CLS"


```
.model large
.code
        public  HOME
HOME    proc
        push    bp
        mov     ax,0200h
        xor     bx,bx
        xor     dx,dx
        int     010h
        pop     bp
        ret
HOME    endp
        end
```

; assembly function to fetch the date for FORTRAN subroutine "getdat(date)"

; integer*4 date


```
.model large
.code
        PUBLIC  gdate
gdate   PROC
```

66

```
        PUSH            BP
        MOV             BP,SP


        xor             AH,AH
        mov             AH,2AH
        int             21H
        les             BX,DWORD PTR [BP+6]
        mov             ES:[BX],DX
        mov             ES:[BX]+2,CX


        POP             BP
        RET             4
gdate   ENDP
        END
```

; assembly function to fetch the time of day for FORTRAN subroutine

; "gettim(time)"

; integer*4 time

```
.MODEL LARGE
.CODE
        PUBLIC  gtime
gtime   PROC
        PUSH            BP
        MOV             BP,SP


        xor             AH,AH
        mov             AH,2CH
        int             21H
        les             BX,DWORD PTR [BP+6]
        mov             ES:[BX],DX
        mov             ES:[BX]+2,CX


        POP             BP
        RET             4
gtime   ENDP
```

```
            END
; assembly function to input a low byte from a port called as FORTRAN
; subroutine "inplb(port,value)"
; integer*4 port,value


.model large
.code
        PUBLIC   INPLB

INPLB   PROC


        PUSH    BP      ;Saves framepointer on stack
        MOV     BP,SP


        LES     BX,DWORD PTR[BP+10]
        MOV     DX,ES:[BX]
        LES     BX,DWORD PTR[BP+6]
        IN      AL,DX
        XOR     AH,AH
        MOV     ES:[BX],AX


        POP     BP      ; Restore the framepointer
        RET     8
INPLB   ENDP
        END
; assembly function to output a low byte to a port called as FORTRAN
; subroutine "outlb(port,value)"
; integer*4 port,value


.model large
.code
        PUBLIC   OUTLB

OUTLB   PROC


        PUSH    BP      ;Saves framepointer on stack
        MOV     BP,SP
```

```
        LES     BX,DWORD PTR[BP+10]

        MOV     DX,ES:[BX]

        LES     BX,DWORD PTR[BP+6]

        MOV     AL,ES:[BX]

        OUT     DX,AL


        POP     BP      ; Restore the framepointer

        RET     8
OUTLB   ENDP

        END
; assembly function to output a character string to the current text

; cursor position.  String must be terminated with a '$' character

; called as a FORTRAN subroutine 'pstrng(c)'

; character c*(up to 80)


.model large

.code

        PUBLIC  pstrng

pstrng  PROC

        PUSH    BP

        MOV     BP,SP


        les     BX,DWORD PTR [BP+6]

        mov     DX,BX

        push    DS

        mov     AX,ES

        mov     DS,AX

        mov     AH,9.

        int     21H

        pop     DS


        POP     BP

        RET     4
pstrng  ENDP
```

```
        END
hcl.obj:    hcl.for
            fl /c hcl.for


hclscrn.obj:    hclscrn.for
            fl /c hclscrn.for


crt_cls.obj:    crt_cls.asm
            masm crt_cls;


crt_home.obj:    crt_home.asm
            masm crt_home;


pstring.obj:    pstring.asm
            masm pstring;


gettime.obj:    gettime.for
            fl /c gettime.for


gtime.obj:    gtime.asm
            masm gtime;


twait.obj:    twait.for
            fl /c twait.for


rdparm.obj:    rdparm.for
            fl /c rdparm.for


stpclr.obj:    stpclr.for
            fl /c stpclr.for


setad.obj:    setad.for
            fl /c setad.for


rdatod.obj:    rdatod.for
```

```
            fl /c rdatod.for


sr9600.obj:    sr9600.for
            fl /c sr9600.for


atodfile.lib:   stpclr.obj setad.obj rdatod.obj sr9600.obj
            lib atodfile -+stpclr.obj -+setad.obj -+rdatod.obj -+sr9600.obj;


sorter.obj:    sorter.for
            fl /c sorter.for


anal01.obj:    anal01.for
            fl /c anal01.for


wait.obj:     wait.for
            fl /c wait.for


pltgr.obj:    pltgr.c
            qcl /c /AL /Od /FPi87 pltgr.c


pltpts.obj:    pltpts.c
            qcl /c /AL /Od /FPi87 pltpts.c


rscreen.obj:   rscreen.c
            qcl /c /AL /Od /FPi87 rscreen.c


keyhit.obj:    keyhit.c
            qcl /c /AL /Od /FPi87 keyhit.c


cfiles.lib:    pltgr.obj pltpts.obj rscreen.obj keyhit.obj
     .       lib cfiles -+pltgr.obj -+pltpts.obj -+rscreen.obj -+keyhit.obj;


inplb.obj:    inplb.asm
            masm inplb;
```

```
outlb.obj:      outlb.asm
            masm outlb;


afiles.lib:     crt_cls.obj crt_home.obj pstring.obj gtime.obj inplb.obj outlb.obj
            lib afiles -+crt_cls.obj -+crt_home.obj -+pstring.obj -+gtime -+inplb.obj -+outlb.obj;


ffiles.lib:     hclscrn.obj twait.obj gettime.obj rdparm.obj sorter.obj anal01.obj wait.obj
            lib ffiles -+hclscrn -+twait -+gettime -+rdparm -+sorter -+anal01 -+wait;


hcl.exe:    hcl.obj
link /NOE hcl,,,ffiles+atodfile+afiles+cfiles+c:quickclib\libc7.lib;
```

APPENDIX C

OPTICAL TRAIN

The optical train of the HCl detector is shown in Figure C.1. Light from the HCl lamp is brought to focus at the center of the rotating matched filter gas cell using a 50 mm focal length calcium fluoride lens and a steering mirror. The HCl lamp is imaged by using a beam stop which limits the aperture to the center portion of the lamp. This stop is placed at the focus of the rear window of the lamp, thus, limiting the off-axis rays from the sidewalls. This beam stop acts as somewhat of an aperture stop for rays in front of the rear window, but does not limit the light from the center of the lamp.

Light passing through the gas cell is then directed by a second steering mirror through a 38 mm f.l. lens to focus the image of the lamp into the White cell. The White cell consists of three mirrors, each having a radius of curvature of 250 mm and arranged in the conventional White cell geometry. The center of curvature of the two rear mirrors have been
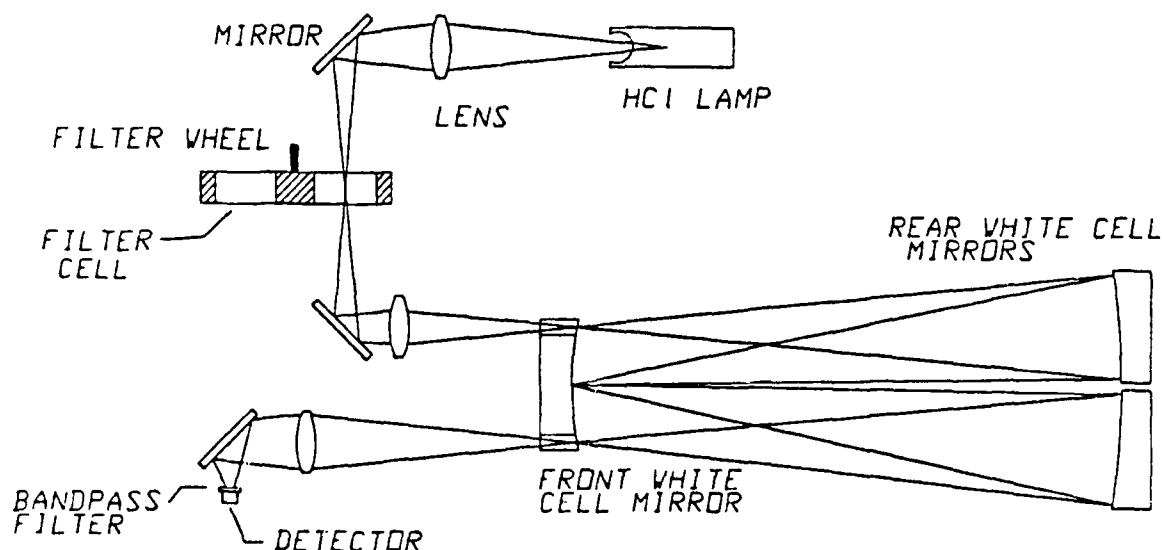
Figure C.1. Schematic of Optical Layout.

machined to be separated by 3 mm. This separation provides six spots, each separated by 6 mm on the top portion of the front mirror before the beam exits off the edge. These spots, together with the seven spots on the bottom portion of the front mirror provide a total of 28 passes through the cell before exiting the other side. Exiting light is passed through a second 38 mm f.l. lens so that the circle of least confusion of the focussed light is centered on the detector by the final steering mirror.

SYSTEM ALIGNMENT

The system is prealigned in the initial assembly. A minimum of realignment should be necessary, and the primary service should involve cleaning the windows and mirrors of the White cell. Access to the White cell is obtained by removing the aerosol heater and dust cover, then removing the 8-32 socket head cap screws from around the cell cover, and sliding the cell cover off. The mirrors can be cleaned with methyl alcohol and a clean cotton swab. However, should a mirror become damaged, realignment must accompany replacement. Since the entire optical train is sealed from the atmospheric sampling area, the primary portion requiring realignment is the White cell mirror assembly, which must be taken out and resurfaced. Each mirror has been plated with a nickel coating, polished and then gold overcoated. When these mirrors are severely contaminated, they should be removed for cleaning and resurfacing.

The White cell field mirrors can be removed as a unit by removing four 6-32 cap screws bolted to the side panels and the two 4-40 flat head cap-screws from the bottom. The entire assembly can thus be cleaned and mirrors resurfaced. Each mirror can also be removed individually; however, much more work would be involved to realign the mirrors, as shims have been placed for final alignment of the White cell due to machining tolerances on the brassboard system. These should be saved for reassembly. The front mirror can be accessed by removing the four 8-32 socket head cap screws next to this mirror. This removes the entire White cell optical bench. Three 6-32 screws also hold this mirror in place. Good nominal alignment

can be achieved by simply rebolting each subsystem back into their original positions. However, if the system has been disassembled, realignment can be achieved as follows:

In order to re-align the optical train, the circulation pump must first be removed. This gives access to the optical axis of the system. Since the lamp is transparent, a small HeNe alignment laser is easily placed in place of the circulation pump to provide a beam of collimated light through the rear end of the lamp. There are a minimum of adjustments within the optical train. Placement of the lenses and mirrors have been machined to nominal positions. Because of machining tolerances in the brassboard instrument; however, some realignment may be necessary when the White cell 's removed and replaced. The optical axis of the system is held at 2.00 inches (50.8 mm) above the optical bench. The laser should, therefore, provide a light beam at this height that is parallel with the optical bench. This laser beam should pass through the left hand slot of the front White cell mirror and fall onto the center of the left rear mirror. The return from this rear mirror should fall directly under the inside edge of the right hand slot. The further passes through the White cell should resemble these shown in Figure C.2. Adjustments of the White cell consists of putting shims under each of the rear mirrors until the two rows of return spots are parallel with the optical bench. Slight adjustments of the rear mirrors can be accomplished by moving these mirrors within their mounting holes before tightening. This "slop" would be keyed out of production instruments.

Once the laser beam exits from the right hand side of the White cell, it should strike the center of the collection lens and be focused onto the detector. Slight misalignments due to non-exact placement of the White cell mirrors may be compensated for by adjusting the steering mirror. Cross adjustments, however, are best made by alignment of the White cell.
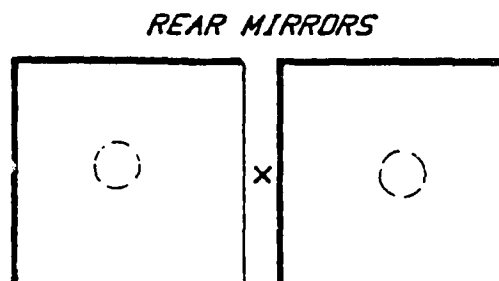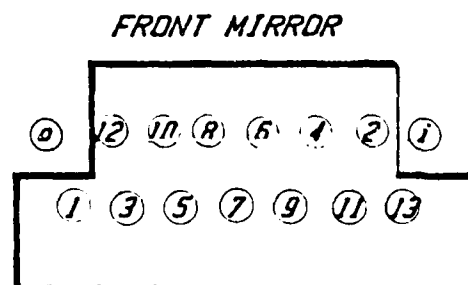
FRONT MIRROR

REAR MIRRORS

Figure C.2.   Schematic of Light Spot Locations on White Cell.

APPENDIX D

ELECTRONIC DESIGN FOR THE HCl MONITOR

The electronic circuits for operating the HCl monitor are physically located in three places:

- within the optical module
- within the power supply module
- inside the portable personal computer

The circuits are briefly described in the following.

A. OPTICAL MODULE ELECTRONICS

Figure D.1 shows the circuits used to amplify and buffer the detector signal, to control the detector refrigeration temperature, to regulate the chopper wheel motor speed, and to regulate the HCl lamp temperature. The aerosol heater operates directly from a 5-volt regulated power supply and does not need control circuitry. It draws a current of about 5 amperes.

All the circuits in the optical module were mounted on a printed circuit board which was soldered to the detector as an integral unit. The power supply and signal paths are provided by an 18-pin military connector.

1. Detector Amplifier and Buffers

The lead selenide detector operates as a photo-conductive device (R_D) with a resistance of 3M ohm. To obtain maximum signal from the detector, the load resistor R_2 is chosen to match this impedance. The signal is AC coupled to a buffer U1a and then amplified by 100 by U1b, and buffered again by U2a. The output of U2a is used to drive the motor controller and the output driver circuit.

Figure D.1.   Circuit Diagram for the Optical Module Electronics.
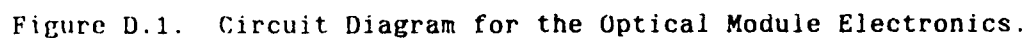
The output driver (U2c, U2d and Q_2) amplifies the signal by 2 and adds to it a positive offset. The latter is necessary to keep the output transistor Q_2 from cut-off. The offset adjustment is done by trimming R10 so that the base line of the output signal is above cut-off (~0.2v above ground). The present circuit can drive 1000 ft of RG-58-u cable with a 50 ohm termination with little signal degradation.

2. Detector Refrigerator Controller

The lead selenide detector is cooled internally by a thermo-electric device. The temperature of the detector is provided by an internal thermister, the calibration curve of which is shown in Figure D.2. To maintain a constant temperature, the current to the thermo-electric cooler R_f is regulated by a negative feedback amplifier composing of U2b and Q_1. The feedback maintains the thermister resistance at 10KΩ which corresponds to a temperature of $-26^{\circ}C$. The circuit has been tested satisfactorily over an environmental temperature range of 20 to $70^{\circ}C$.

3. Motor Speed Controller

The detector signal from buffer U2a is filtered by R30 and C13 and AC coupled into the frequency to voltage converter U3. The converted voltage is compared with a reference voltage set by R19, and the difference signal is used in a feedback loop to maintain the motor speed. Different motor speeds may be obtained by adjustment of R19. The normal speed is set at ~1900 rpm.
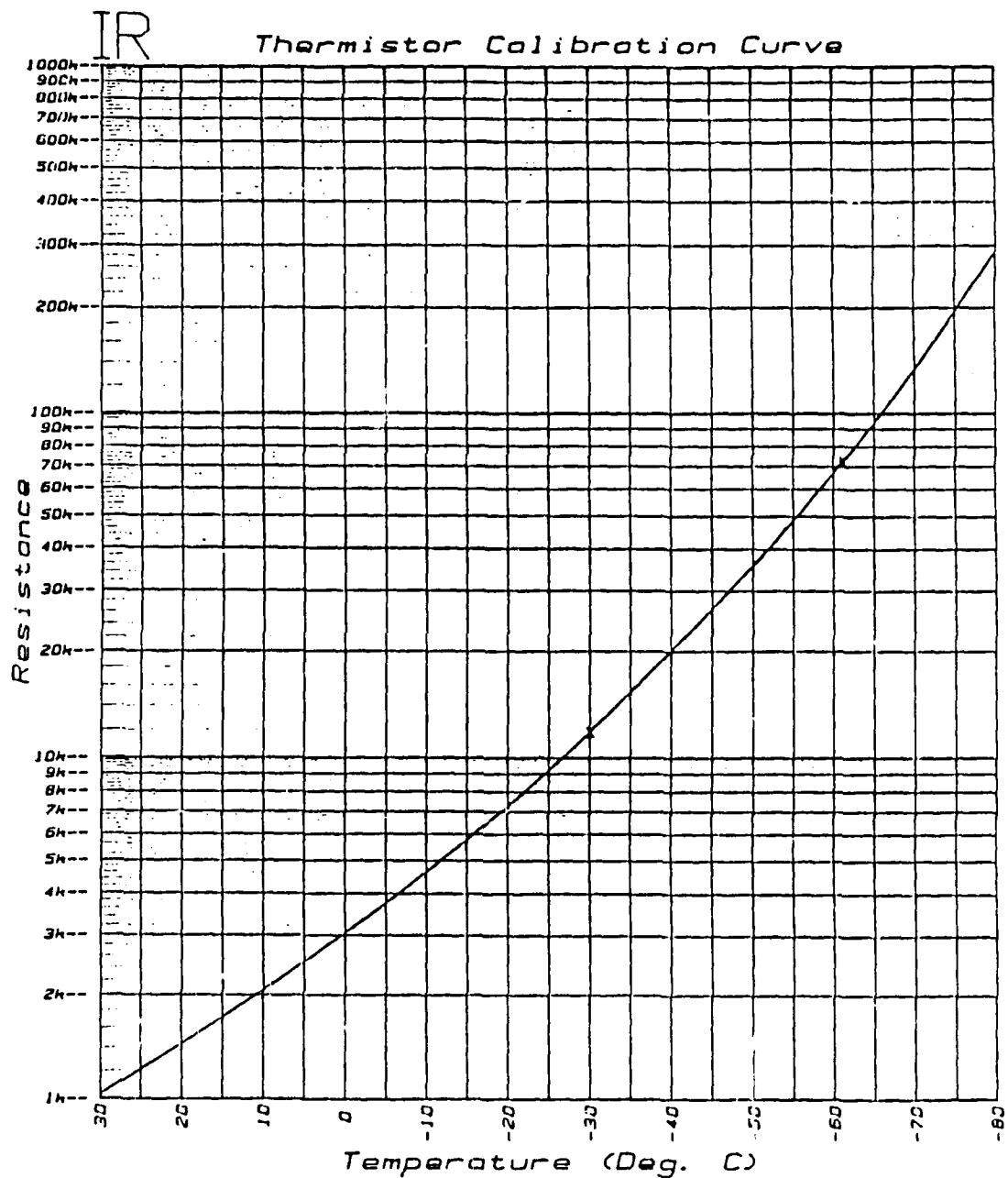
Figure D.2. Calibration Curve of Thermistor in the PbSb Detector.

4. The HCl Lamp Temperature Controller

The temperature of the HCl lamp is measured by a Type K thermocouple located at about the middle of the lamp. The thermocouple voltage is amplified by U4 (which also provides an ice-point internal reference). This voltage is compared with a preset value set by R29. The difference is used to drive the feedback amplifier U5a and Q_4 to provide the necessary lamp current for stable temperature operation. The temperature to voltage transfer function for U4 is given in the following table.

$\underline{T}$(C)	$\underline{V}$(Volts)	
500	5.107	
600	6.101	
700	7.206	(source: Analog
800	8.232	Devices Data Book)
900	9.233	

A typical lamp temperature history is shown in Figure D.3. The heat up process started at A. (The lamp was slightly hotter than room temperature because it had not cooled down completely from a previous test.) The heat up time (to B) was about 3 1/2 minutes with a slight temperature overshoot at B. At C, the temperature set point was readjusted (by adjustment of R29), and the lamp temperature increased to D. The temperature remained constant for the rest of the test period.

B. POWER SUPPLY MODULE

The power supply module houses five regulated power supplies (see Figure D.4). The 100-volt low current supply for the detector was regulated by a zener diode. The other four supplies were commercial units. The 25-volt supply was a 28-volt commercial unit adjusted down to 25 volt. The AC line current was about 2 amperes.
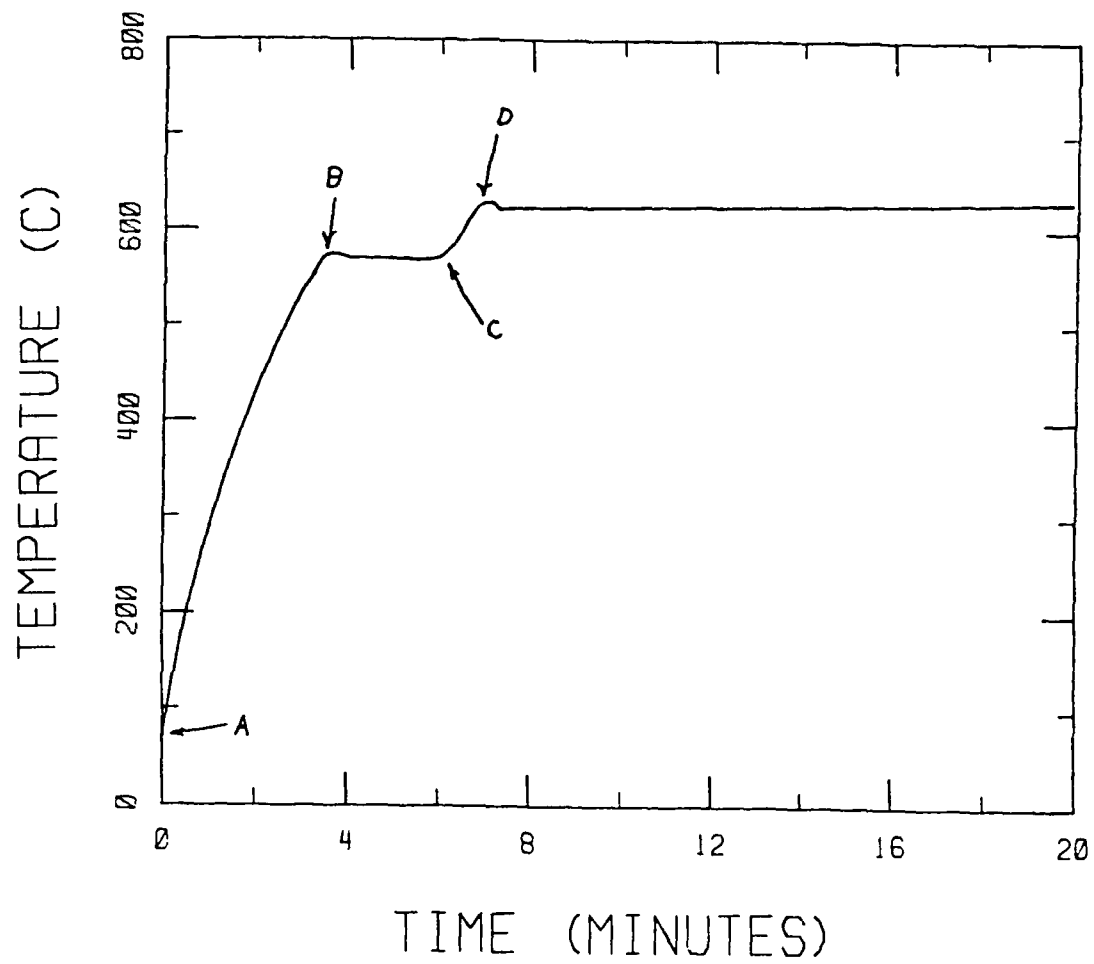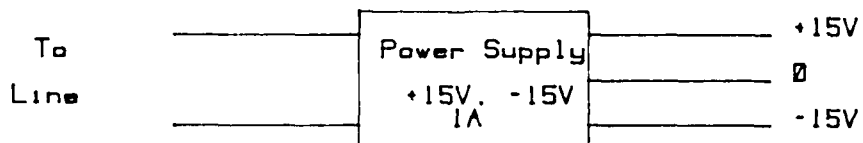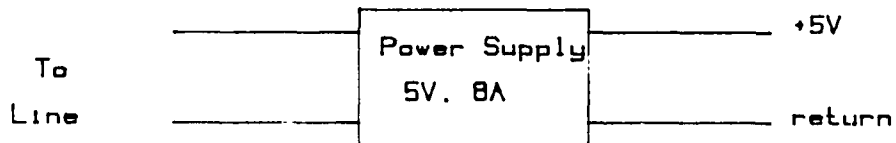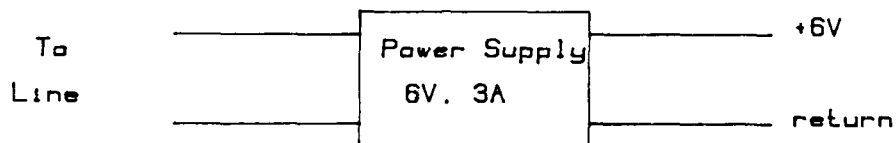
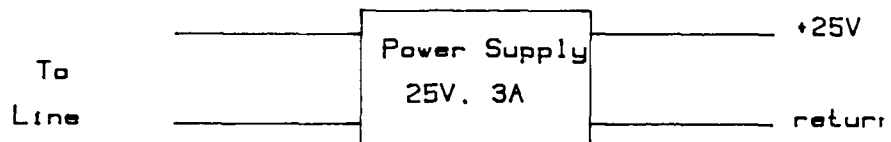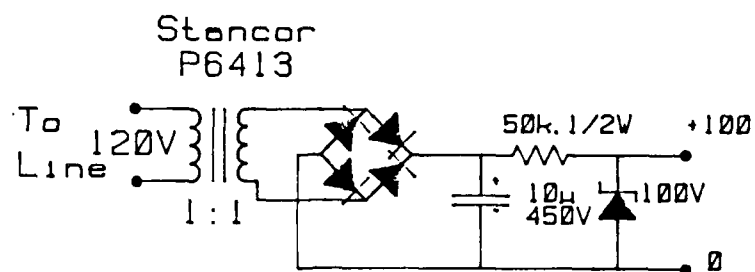Figure D.3.   HCl Lamp Temperature History.

Figure D.4.   Power Supply Module.

C. COMPUTER MODULE

The computer module consists of a Compaq portable PC-XT compatible personal computer. The analog to digital conversion is performed by a Data-Translation DT 2812 board. The signal from the HCl monitor is buffered by the circuit shown in Figure D.5. Also shown on the figure is the circuit which derives a clock signal from the analog signal to strobe in the data.

Referring to Figure D.5, the analog signal is filtered by R102 and C102, buffered by U101b, and is then fed to the analog input of the A to D converter. The clock signal is derived from the analog signal using a Schmidt trigger (U101c), the output of which is inverted by Q101 and connected to the monostable multivibrators U102 and U103. The time delay of the trigger signals (which can be measured at pin 5 of U102b and U103b) from the trailing edge of the signal (at the inputs (pin 1) of U102a and U103a) are set by R109 and R112,respectively. The timing diagram is shown at the bottom of Figure D.5. The trigger signals are combined by a NOR gate (U104) and inverted by Q102 to provide the strobe signal for the A to D conversion.

The +12-, -12-, and +5-volt power supplies for the above circuit were obtained from the bus connector of the computer.

D. ADJUSTMENTS

The adjustments within the optical module are:
- Lamp temperature adjustment R29.
- Motor speed adjustment R19.
- Signal offset adjustment R11.

The locations of these adjustment trim pots are shown in Figure D.6. The adjustments within the computer module are:
- Time delay adjustment for the signal strobe R109.
- Time delay adjustment for the baseline strobe R112.

The location of these adjustment trim pots are shown in Figure D.7.
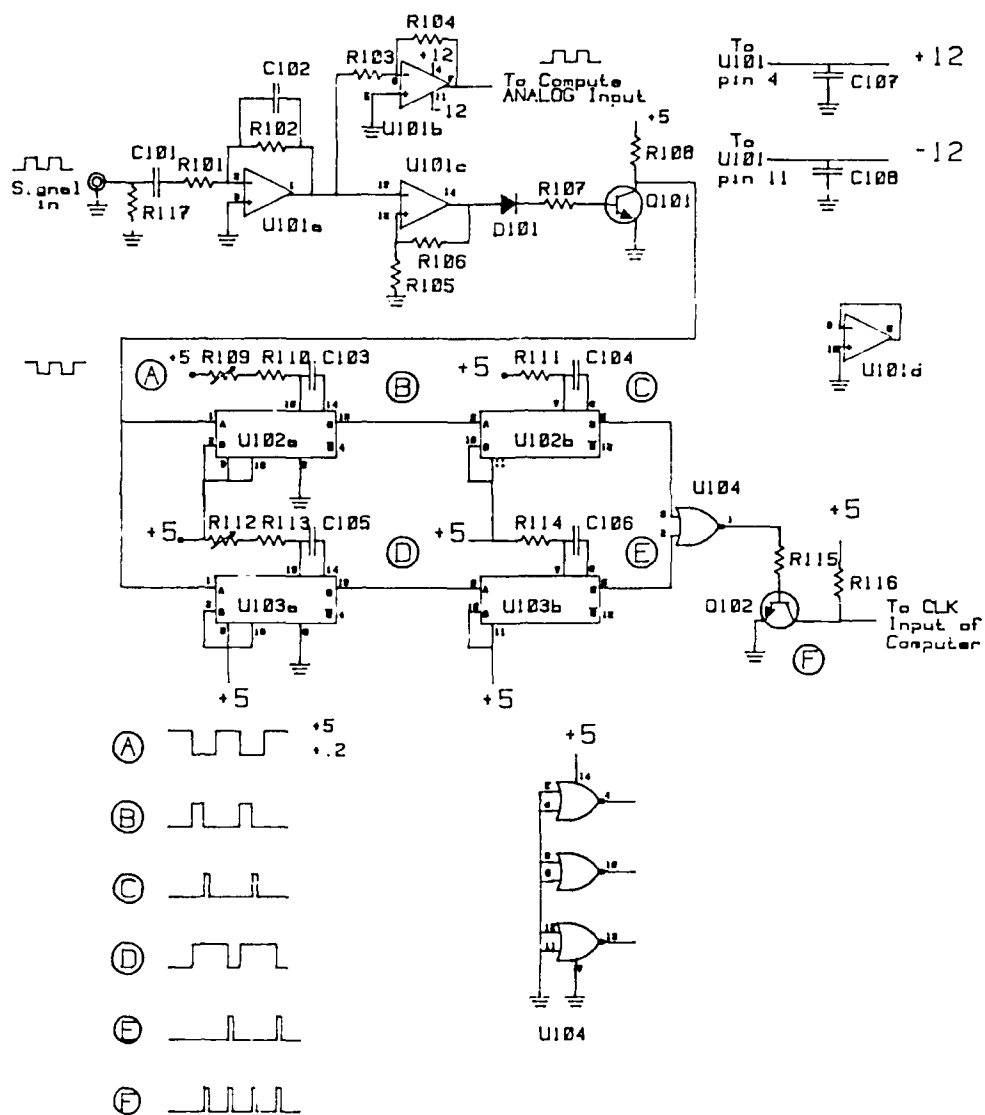
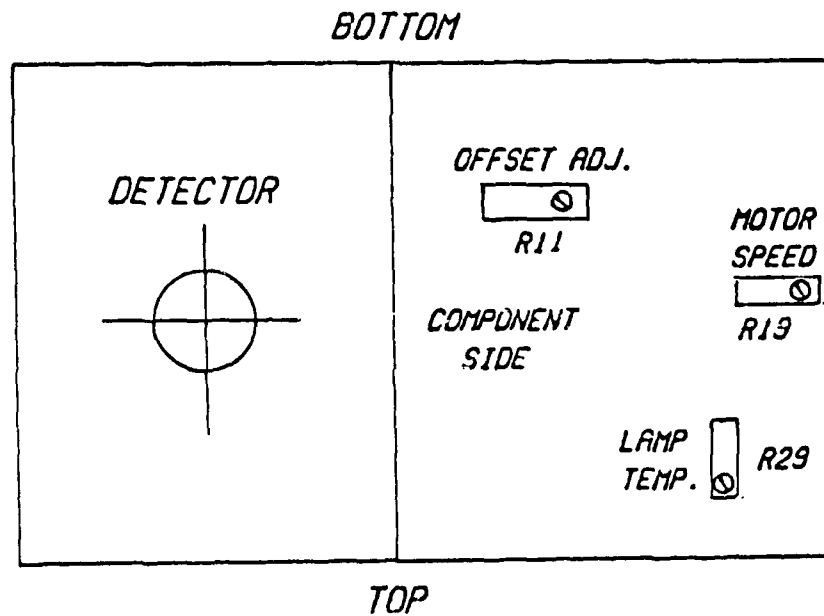Figure D.5.   Signal Buffer and Strobe Generator Within the Computer Module.

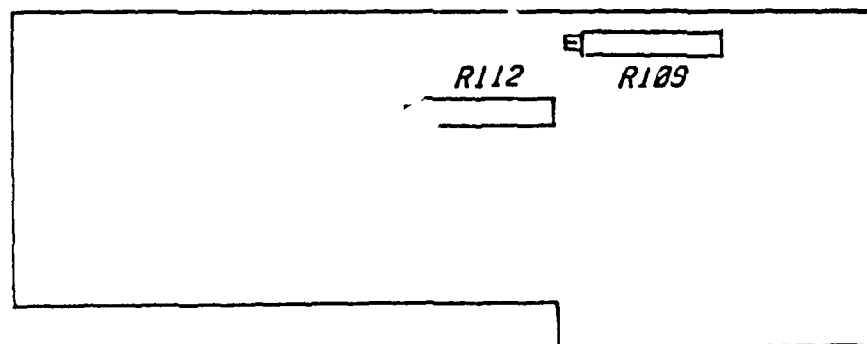Figure D.6.   Adjustments on PC Board Within the Optical Module.

Figure D.7.   Adjustments on PC Board Within the Computer Module.